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On the elastic scattering of neutrons by deuterons

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Introduction.

The knowledge of the interaction potential between two nucleons is of fundamental importance in nuclear physics, and every experimental result giving a clue to it is of great interest.

Especially important are the collision experiments which concern two nucleons and those concerning the bound states of the deuteron. These serve most directly to limit the theoretical possibilities for the nucleon-nucleon potential, because the processes involving more than two nucleons are so difficult from the mathetical point of view, that one is forced to make use of simplifications which are perhaps not fully justified. The difficulties involved in connection with the so called "many body forces" are also avoided by dealing with only two-nucleon systems.

The charge independence and short range of the nuclear forces are now rather well established facts. On the other hand, the so called "exchange" character of the forces remains (apart from preliminary experiments on proton-proton scattering) an open question.

The potential (between two nucleons, 2 and 3) may be either of the form

$$-U_{23}\left\{\left(1-\frac{1}{2}g\right)+\frac{1}{2}g\,(\boldsymbol{\sigma}^{(2)}\cdot\boldsymbol{\sigma}^{(3)})\right\} \tag{1}$$

which is suggested by neutral meson theory, or

$$+\frac{1}{3}U_{23}\,(\boldsymbol{\tau}^{(2)}\cdot\boldsymbol{\tau}^{(3)})\cdot\left\{\left(1-\frac{1}{2}g\right)+\frac{1}{2}g\,(\boldsymbol{\sigma}^{(2)}\cdot\boldsymbol{\sigma}^{(3)})\right\} \tag{2}$$

which is suggested by the symmetrical meson theory.

The two body scattering experiments have not yet been able to distinguish definitely between these two possibilities. One reason for this is that when the P-wave scattering becomes important the above static forces are no longer permissible. The proton-deuteron

(P-D) or the neutron-deuteron (N-D) scattering on the other hand, is suitable to this purpose because the large size of the deuteron gives an appreciable P-wave scattering for relatively small energies (a few MeV). The experimental curves for the angular dependence of the P-D scattering for proton energies from 1.5 to 3.5 MeV[1]) and for the N-D scattering for a neutron energy of 2.5 MeV[2]), have in common a strong maximum at 180° in the center of mass system. This maximum becomes more pronounced with increasing P. energy.

An adequate theory must be able to furnish on the basis of these experimental results arguments for one of the two potentials given above[10]).

The purpose of this paper is to present a theory of the N-D scattering. The three main results are:

1. Rigorous treatment of spin and isotopic spin.
2. The generalization of the well known integral form for the scattering phases for the case of three particles.
3. The extension of the variational method for the calculation of these phases, which has already been successfully applied by Hulthén[3]) for the two-body problem.

Inspection of these exact integral formulae allows one to draw conclusions about the exchange nature of the forces.

A detailed comparison with experiment is unfortunately not possible because the experimental results on N-D scattering are rather poor. On the other hand those for P-D scattering are excellent, and a theoretical investigation of this more complicated problem is now under way.

I. Interaction and equations of motion.

Our considerations apply to any potential between two bodies 2 and 3 which have the form

$$V_{23} = U_{23} \cdot \{w \cdot + b(23)_\sigma + h(23)_\tau + m(23)_{\sigma\tau}\} \tag{3}$$

where w, b, h, m are constants. (23) is the permutation of the spacial coordinates of 2 and 3 and $(23)_\sigma$ is the permutation of coordinates of spin, $(23)_\tau$ that of isotopic spin and $(23)_{\sigma\tau}$ is simultaneously the permutation of the spin and isotopic spin of the particles 2 and 3. U_{23} depends only on the distance between 2 and 3.

Since

$$(\boldsymbol{\sigma}^{(2)} \cdot \boldsymbol{\sigma}^{(3)}) = 2(23)_\sigma - 1 \qquad (\boldsymbol{\tau}^{(2)} \cdot \boldsymbol{\tau}^{(3)}) = 2 \cdot (23)_\tau - 1$$

the two interactions 1) and 2) are particular cases of this type.

In the three body problem an important part is played by the symmetry operators T^s, T', T'' which are defined as follows

$$\left.\begin{aligned} T^s &= (23) + (13) + (12) \\ T' &= \frac{\sqrt{3}}{2}\{(13) - (12)\} \\ T'' &= -(23) + \frac{1}{2}\{(13) + (12)\} \end{aligned}\right\} \tag{4}$$

These operators can operate on a single species of coordinates, i. e. on the spacial, spin or isotopic spin coordinates, or act at the same time at both spin and isotopic spin coordinates. This will be indicated by a subscript, as already used in (3) for the simple permutation.

Applied to a function symmetric in the coordinates of 2 and 3, these three operators generate three functions, the first of which is completely symmetrical in the coordinates of 1, 2, 3, while the other two functions transform by permutation of two of the coordinates, 1, 2, 3, according to the two-dimensional unitary representation D.

$$(12) = \begin{pmatrix} 1/2 & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -1/2 \end{pmatrix} \qquad (23) = \begin{pmatrix} -1 & 0 \\ 0 & +1 \end{pmatrix} \qquad (13) = \begin{pmatrix} 1/2 & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -1/2 \end{pmatrix}$$

Thus for example, if one operates on the spacial potential U_{23}, the three following potentials are obtained

$$\left.\begin{aligned} U^s &= T^s\, U_{23} = U_{23} + U_{21} + U_{13} \\ U' &= T'\, U_{23} = \frac{\sqrt{3}}{2}(U_{21} - U_{13}) \\ U'' &= T''\, U_{23} = -U_{23} + \frac{1}{2}(U_{21} + U_{13}) \end{aligned}\right\} \tag{5}$$

of these U^s is completely symmetrical in 1, 2, 3 and U', U'' transform according to the representation D. In particularly U' is antisymmetrical in 2, 3, while U'' is symmetrical. If the distance of particle 1 to particles 2 and 3 increases, the potential U' goes rapidly to zero, whereas U'' reduces to $-U_{23}$. It may be readily proved that the potentials U^s, U', U'' are mutually orthogonal, i. e.

$$\int U^s \cdot U'\, dv = \int U^s \cdot U''\, dv = \int U' \cdot U''\, dv = 0$$

where $dv = d^3 r_1\, d^3 r_2\, d^3 r_3$ is the volume element in the space of the nucleon coordinates $\vec{r}_1$, $\vec{r}_2$, $\vec{r}_3$. The integrals are extended over all space.

Assuming the addivity of the potentials, the total interaction of the three bodies may now be written:

$$W = U^s O^s + U' O' + U'' O'' \tag{6}$$

where the operators O operate on the spin and isotopic spin coordinates only and are defined as follows

$$\left.\begin{aligned} O^s &= \frac{1}{3}(bT^s_\sigma + hT^s_\tau + mT^s_{\sigma\tau}) + w \\ O' &= -\frac{2}{3}(bT'_\sigma + hT'_\tau + mT''_{\sigma\tau}) \\ O'' &= +\frac{2}{3}(bT''_\sigma + hT''_\tau + mT''_{\sigma\tau}) \end{aligned}\right\} \tag{7}$$

Three body potentials, i. e. potentials depending simultaneously on the coordinates of the three nucleons, the existence of which is as yet not established, could be treated by the formalism just described; one would have only to change the significance of U^s, U' and U''.

The next step is to find in the spin and isotopic spin space a basis in which the operators O are represented by irreducible matrices.

Both spin and isotopic spin of the nucleons have the values 1/2. Hence the total spin S and the total isotopic spin T of three nucleons can assume the values 3/2 and 1/2. Four eigenfunctions χ^s belong to $S = 3/2$ and to $S = 1/2$ another four eigenfunctions, namely two pairs (χ'_+, χ''_+) and (χ'_-, χ''_-), each of which can be chosen in such a way that as to transform by permutations according to the representation D.

To obtain for instance the pair (χ'_+, χ''_+) which corresponds to $S_z = 1/2$, one has to operate with T'_σ and T''_σ on the symmetrical spin eigenfunction

$$\chi_{23} = \sqrt{\frac{2}{3}}(\alpha_2\beta_3 + \alpha_3\beta_2)\cdot\alpha_1$$

where

$$\begin{cases} \sigma_z^{(1)}\alpha_1 = \alpha_1 \\ \sigma_z^{(1)}\beta_1 = -\beta_1 \end{cases}$$

The same applies for the isotopic spin eigenfunctions. To the total isotopic spin $T = 3/2$ belong four symmetrical eingenfunctions ζ^s, and to the spin $T = 1/2$ the two pairs (ζ'_+, ζ''_+) and (ζ'_-, ζ''_-), which may be obtained in the same way as the corresponding spin eingenfunctions.

The functions χ^s, (χ', χ''); ζ^s, (ζ', ζ'') are mutually orthogonal and normalized. In the product space of spin and charge (for $S = T = 1/2$), the direct product representation $D \times D$ decomposes into a sum of three representations[4)][5)], viz.

$$D \times D = I + A + D$$

a completely symmetrical one I, a completely antisymmetrical one A, and a two-dimensional one D. Therefore, one can choose in the product space of spin and charge, for $S = T = 1/2$, the basis

$$\xi^s = \frac{1}{\sqrt{2}} \cdot (\chi'\zeta' + \chi''\zeta''), \qquad \xi^a = \frac{1}{\sqrt{2}} (\chi'\zeta'' - \chi''\zeta'),$$
$$\xi' = \frac{1}{\sqrt{2}} (\chi'\zeta'' + \chi''\zeta'), \qquad \xi'' = \frac{1}{\sqrt{2}} (\chi'\zeta' - \chi''\zeta'')$$

of which the ξ'_s are orthogonal eingefunctions normalized to unity. The latter transform under permutation of the variables according to the corresponding representation I, A, and D.

As the interaction W is an invariant with respect to rotation in spin and isotopic spin space, the total spin and the total isotopic spin are constants of motion. Only the case in which the isotopic spin $T = 1/2$ has to be taken into account for N-D scattering, because the deuteron is antisymmetrical in the charge in its ground state. The isotopic spin eigenfunctions are therefore

$$\zeta'_- = T'_\tau \cdot \left\{ \sqrt{\frac{2}{3}} (b_2 a_3 + a_2 b_3) a_1 \right\} \qquad \text{where} \quad \begin{cases} \tau_z^{(1)} a_1 = a_1 \\ \tau_z^{(1)} b_1 = -b_1 \end{cases}$$
$$\zeta''_- = T''_\tau \cdot \left\{ \sqrt{\frac{2}{3}} (b_2 a_3 + b_3 a_2) a_1 \right\}$$

They correspond to a total charge

$$\varepsilon = e \cdot \left[\frac{3}{2} + \frac{1}{2} \sum \tau_z \right]$$

equal to e.

Hence, the total eigenfunction may be written as follows

$$\left.\begin{aligned} &\text{for } S = \frac{3}{2} \qquad \psi = (\psi'\zeta'' - \psi''\zeta') \cdot \chi^s \\ &\text{for } S = \frac{1}{2} \qquad \psi = \psi^a \xi^s - \psi^s \xi^a + \psi' \xi'' - \psi'' \xi' \end{aligned}\right\} \qquad (8)$$

$(\psi' \cdot \psi'')$ and (ψ^s, ψ^a) depend on the spacial coordinates only. To statisfy the Paui principle, ψ^s must be totally symmetrical, ψ^a otally antisymʟmetrical and finally (ψ', ψ'') must transform according to the D respresentation. We notice, in particular, that ψ' is antisymmetrical in 2 and 3, while ψ'' is symmetrical in these coordinates.

The operators T', T'' are represented in the space of $(\chi^s \zeta', \chi^s \zeta'')$ by

$$\left.\begin{array}{lll} T^s_\sigma = 3 & T^s_\tau = 0 & T^s_{\sigma\tau} = 0 \\ T'_\sigma = 0 & T'_\tau = -\frac{3}{2}\sigma_1 & T'_{\sigma\tau} = -\frac{3}{2}\sigma_1 \\ T''_\sigma = 0 & T''_\tau = \frac{3}{2}\sigma_3 & T''_{\sigma\tau} = \frac{3}{2}\sigma_3 \end{array}\right\} \tag{9}$$

where σ_1, σ_2, σ_3 are the usual two-dimensional PAULI matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

In the product space of the $\xi's$ one has

$$\left.\begin{array}{lll} T^s_\sigma = 0 & T^s_\tau = 0 & T^s_{\sigma\tau} = 3\begin{pmatrix} \sigma_3 & 0 \\ 0 & 0 \end{pmatrix} \\ T'_\sigma = -\frac{3}{2}\cdot\begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix} & T'_\tau = -\frac{3}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & T'_{\sigma\tau} = -\frac{3}{2}\begin{pmatrix} 0 & 0 \\ 0 & \sigma_1 \end{pmatrix} \\ T''_\sigma = +\frac{3}{2}\begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix} & T''_\tau = +\frac{3}{2}\begin{pmatrix} 0 & i\sigma_2 \\ -i\sigma_2 & 0 \end{pmatrix} & T''_{\sigma\tau} = \frac{3}{2}\begin{pmatrix} 0 & 0 \\ 0 & \sigma_3 \end{pmatrix} \end{array}\right\} \tag{10}$$

these matrices having four rows and columns. The operators T form, for three-body problems, a most natural generalization of the usual exchange operators.

For the operators O defined by (7) one has for $S = 3/2$

$$\left.\begin{array}{l} O^s = w + b \\ O' = (h + m)\cdot\sigma_1 \\ O'' = (h + m)\cdot\sigma_3 \end{array}\right\} \tag{11}$$

for $S = 1/2$

$$O^s = w + \begin{pmatrix} m\sigma_3 & 0 \\ 0 & 0 \end{pmatrix} \quad O' = \begin{pmatrix} 0 & h + b\sigma_3 \\ h + b\sigma_3 & m\sigma_1 \end{pmatrix} \quad O'' = \begin{pmatrix} 0 & b\sigma_1 + ih\sigma_2 \\ b_1\sigma - ih\sigma_2 & m\sigma_3 \end{pmatrix} \tag{12}$$

In the SCHROEDINGER equation of our problem

$$(E - T)\,\psi = W\,\psi$$

E is the total energy, equal to the sum

$$E = E_k - E_d$$

where E_k is the kinetic energy of the impinging neutron and $-E_d = -2.19$ MeV the binding energy of the deuteron; T the operator for the total kinetic energy, viz:

$$T = T_1 + T_2 + T_3 = -\frac{\hbar^2}{2M}\cdot(\Delta_1 + \Delta_2 + \Delta_3)$$

We have chosen as spacial coordinates those generated by operating with the usual symmetry-operators T on one of the nucleon radius vector, e. g. $\vec{r}_1$

$$\left.\begin{aligned} \vec{q}^s &= \frac{1}{3} T^s \vec{r}_1 = \frac{1}{3}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3) \\ \vec{r} &= \quad T' \vec{r}_1 = \frac{\sqrt{3}}{2}(\vec{r}_3 - \vec{r}_2) \\ \vec{q} &= \quad T'' \vec{r}_1 = -\vec{r}_1 + \frac{1}{2}(\vec{r}_3 + \vec{r}_2) \end{aligned}\right\}$$

$\vec{q}^s$ is the center of mass (C. M.) coordinate, $\vec{r}$ is proportional to the distance of 2 from 3, and $\vec{q}$ is the distance of nucleon 1 from the C. M. of 2 and 3. Any pair of components of the two vectors $\vec{r}$ and $\vec{q}$ transforms according to D. The volume element $d\tau = d^3 r \cdot d^3 q$ is invariant with respect to permutation of 1, 2, 3. In this coordinate system, the kinetic energy has the form

$$T = -\frac{\hbar^2}{2M} \Delta_{qs} - \frac{3\hbar^2}{4M}(\Delta_r + \Delta_q)$$

In the C. M. system, which moves with respect to the rest system with a kinetic energy $E_s = \frac{1}{3} E_k$, putting

$$k^2 = \frac{8}{9} \frac{M}{\hbar^2} E_k \qquad k_d^2 = \frac{4}{3} \frac{M}{\hbar^2} E_d$$

the Schroedinger equation reads:

$$(\Delta_r + \Delta_q + k^2 - k_d^2)\,\psi = \frac{4}{3}\frac{M}{\hbar^2}(U^s O^s + U' O' + U'' O'')\,\psi \tag{13}$$

Eliminating the spin and isotopic spin coordinates, by means of (11) and (12) one obtains the following systems of differential equations for the spacial wave functions:

$$\text{for } S = \frac{3}{2} \quad \left.\begin{aligned} \mathfrak{T}\psi' &= (w+b)\,U^s\psi' - (h+m)\cdot(U'\psi'' + U''\psi') \\ \mathfrak{T}\psi'' &= (w+b)\,U^s\psi'' - (h+m)\cdot(U'\psi' - U''\psi'') \end{aligned}\right\} \tag{14}$$

for $S = \frac{1}{2}$

$$\left.\begin{aligned} \mathfrak{T}\psi^a &= (w+m)\,U^s\psi^a - (b+h)\,(U'\psi'' - U''\psi') \\ \mathfrak{T}\psi^s &= (w-m)\,U^s\psi^s + (b-h)\,(U''\psi'' - U'\psi') \\ \mathfrak{T}\psi' &= (b+h)\,U''\psi^a + (b-h)\,U'\psi^s - m\,(U'\psi'' + U''\psi') + w\,U^s\psi' \\ \mathfrak{T}\psi'' &= -(b+h)\,U'\psi^a + (b-h)\,U''\psi^s + m\,(U''\psi'' - U'\psi') + w\,U^s\psi'' \end{aligned}\right\} \tag{15}$$

*

From now on all the potentials are understood to be multiplied by $\frac{4}{3}\frac{M}{\hbar^2}$ and $\mathfrak{T}$ stands for the operator

$$\mathfrak{T} = \Delta_r + \Delta_q + k^2 - k_d^2 \tag{16}$$

In our coordinate system the total angular momentum is given by

$$\frac{\hbar}{i}\Sigma[\vec{r}_\varkappa \cdot \vec{\nabla}_{r_\varkappa}] = \frac{\hbar}{i}\{[\vec{r}\cdot\vec{\nabla}_r] + [\vec{q}\cdot\vec{\nabla}_q]\}.$$

This operator commutes with $\mathfrak{T}$. As further the potentials U belong to a total angular momentum zero, any one of the equations forming the systems admits the group of the rotations in the space of $\vec{r}$ and $\vec{q}$. Every component ψ belong therefore to a given total angular momentum.

For our collision problem one must now satisfy the following requirements:

a) for $S = 3/2$, a solution ψ', ψ'' of the system (14) must be found such that ψ' go rapidly to zero as nucleon 1 leaves the ranges of interaction of 2 and 3, while ψ'' has for large $q's$ the following asymptotic behaviour

$$\psi'' \simeq \varphi(r)\left(e^{ikq\cos\vartheta} + f^{(\frac{3}{2})}(\vartheta)\frac{e^{ikq}}{q}\right) \tag{17}$$

$\varphi(r)$ is the eigenfunction of the deuteron in the ground state and ϑ is the angle by which the impinging neutron is scattered.

b) for $S = 1/2$ a solution ψ^s, ψ^a, ψ', ψ'' of the system (15) must be found such that (ψ^a, ψ') go to zero for large $q's$, and ψ^s, ψ'' behave asymptotically as follows

$$\left.\begin{aligned} \psi^s &\cong +\frac{1}{\sqrt{2}}\varphi(r)\left(e^{ikq\cos\vartheta} + f^{(1/2)}(\vartheta)\frac{e^{ikq}}{q}\right) \\ \psi'' &\simeq -\frac{1}{\sqrt{2}}\varphi(r)\cdot\left(e^{ikq\cos\vartheta} + f^{(1/2)}(\vartheta)\frac{e^{ikq}}{q}\right) \end{aligned}\right\} \tag{18}$$

In fact the deuteron must be left, once the neutron is elastically scattered, in its ground state. This corresponds to the spin and isotopic spin eigenfunction

$$\chi''\zeta' = \frac{1}{\sqrt{2}}(\xi' - \xi^a)$$

For evaluating the total cross-section $\sigma(\vartheta)$ one needs only to know the functions $f^{(3/2)}(\vartheta)$, $f^{(1/2)}(\vartheta)$ being

$$\sigma(\vartheta) = \frac{2}{3}|f^{(\frac{3}{2})}(\vartheta)|^2 + \frac{1}{3}|f^{(1/2)}(\vartheta)|^2 \tag{19}$$

II. Integral relation for the determination of the phases.

The equation of motion, written in the form (14), (15) makes it possible to generalize, for the three-body case, well known integral relations[6]) which gives the phases of the scattered waves in two-body problems.

Let us put

$$I_l^+ = \sqrt{\frac{\pi}{2\,k\,q}}\,J_{l+1/2}(k\,q), \qquad I_l^- = (-1)^l \sqrt{\frac{\pi}{2\,k\,q}}\,J_{-l-1/2}(k\,q)$$

where $J_{l+1/2}(k\,q)$ and $J_{-l-1/2}(k\,q)$ are Bessel functions of order $l+1/2$ and $-l-1/2$ respectively. One has then for large $q's$

$$I_l^+ \simeq \frac{\sin(k\,q - l\,\pi/2)}{k\,q} \qquad I_l^- \simeq \frac{\cos(k\,q - l\,\pi/2)}{k\,q}$$

By a known property of these functions, one has furthermore

$$I_l^- \frac{\partial I_l^+}{\partial q} - I_l^+ \frac{\partial I_l^-}{\partial q} = \frac{1}{k\,q^2} \tag{20}$$

Calling φ_l^+, φ_l^- the two functions defined as follows

$$\left.\begin{aligned} \varphi_l^+(r, q) &= \varphi(r)\cdot i^l\,(2\,l+1)\,e^{i\,\delta_l}\quad I_l^+(k\,q)\cdot P_l(\cos\vartheta_q) \\ \varphi_l^-(r, q) &= \varphi(r)\cdot i^l\,(2\,l+1)\,e^{i\,\delta_l}\quad I_l^-(k\,q)\cdot P_l(\cos\vartheta_q) \end{aligned}\right\} \tag{21}$$

where $\vec{q}\cdot\vec{k} = q\cdot k\,\cos\vartheta_q$ and P_l is the Legendre polynomial of order l. Denoting by Ω the operator

$$\Omega = \mathfrak{T} + U_{23} = \Delta_r + \Delta_q + k^2 - k_d^2 + U_{23}$$

one has

$$\left.\begin{aligned} \Omega\,\varphi_l^+ &= 0 \\ \Omega\,\varphi_l^- &= 0 \end{aligned}\right\}$$

We shall now prove that the following formula

$$\sin\,\delta_l = \frac{k}{4\,\pi}\cdot\frac{1}{2\,l+1}\int \varphi_l^{+*}\,\Omega\,\psi\,d\,\tau \tag{22}$$

applies to any function which is regular over all space and which behaves asymptotically with respect to q

$$\psi \simeq -(\varphi_l^+ \cos\delta_l + \varphi_l^- \sin\delta_l)$$

In order to show this, let us integrate, in the space of $\vec{r}$ and $\vec{q}$, the following identity:

$$\begin{aligned} \varphi_l^{+*}\,\Omega\,\psi - \psi\,\Omega\,\varphi_l^{+*} &= \varphi_l^{+*}\,(\Delta_r + \Delta_q)\,\psi - \psi\,(\Delta_r + \Delta_q)\,\varphi_l^{+*} = \\ &= \mathrm{Div}_r\,(\varphi_l^{+*}\nabla_r\,\psi - \psi\,\nabla_r\,\varphi_l^{+*}) + \mathrm{Div}_q\,(\varphi_l^{+*}\,\nabla_q\,\psi - \psi\,\nabla_q\,\varphi_l^{+*}) \end{aligned}$$

taking into account that φ_l^+ and $\nabla_r \varphi_l^+$ go for large $\vec{r}$ rapidly enough to zero and making use of the relation (20); $\varphi(r)$ is understood to be normalized as follows

$$\int |\varphi(r)|^2 d^3 r = 1 \tag{23}$$

Starting from the identity

$$\varphi_l^{-*} \Omega \psi - \psi \Omega \varphi_l^{-*} = \mathrm{Div}_r (\varphi_l^{-*} \nabla_r \psi - \psi \nabla_r \varphi_l^{-*}) + \mathrm{Div}_q (\varphi_l^{-*} \nabla_q \psi - \psi \nabla_q \varphi_l^{-*})$$

we obtain in analogous way a similar relation for the cos of the phases:

$$(\omega_l - 1) \cos \delta_l = \frac{k}{4\pi} \cdot \frac{1}{2l+1} \cdot \int (\varphi_l^{-*} \Omega \psi - \psi \Omega \varphi_l^{-*})\, d\tau \tag{24}$$

where ω_l is a constant as defined by

$$\omega_l = \lim_{q \to 0} \frac{k}{4\pi} \cdot \frac{1}{2l+1} \cdot \int \left(\varphi_l^{-*} \frac{\partial \psi}{\partial q} - \psi \frac{\partial \varphi_l^{-*}}{\partial q} \right) d^3 r\, d\omega_q \cdot q^2 \tag{25}$$

This constant is finite only if ψ vanishes rapidly enough for small values of q. $\varphi(r)$ is here again supposed to be normalized according to (23). We can now apply the integral relation (22) and (24) to the particular case of a solution of the systems of differential equations (14), (15) discussed in the preceding section, as these solutions are of the required form. These systems of equations yield likewise $\Omega \psi$ as function of the potentials and the same ψ's.

For $S = 3/2$ it is the function ψ'' corresponding to a given angular momentum which has the right asymptotic behaviour, while in the case of $S = 1/2$, for the same reason, the linear combination

$$\psi = \frac{1}{\sqrt{2}} (\psi'' - \psi^s)$$

must be used. One has
for $S = 3/2$

$$\Omega \psi'' = \left(w + b + \frac{h+m}{2} \right) \overline{U} \psi'' - (h+m) U' \psi' \tag{26}$$

for $S = 1/2$

$$\Omega \psi = \left\{ \left(w + \frac{m}{2} - \frac{b-h}{2} \right) \frac{\psi''}{\sqrt{2}} - \left(w - m - \frac{b-h}{2} \right) \frac{\psi^s}{\sqrt{2}} \right\} \cdot \overline{U}$$
$$- \left\{ (b - h + m) \frac{\psi'}{\sqrt{2}} + (b+h) \frac{\psi^a}{\sqrt{2}} \right\} U', \tag{26$'$}$$

where $\overline{U} = U_{13} + U_{23}$

Consequently, the following rigorous integral formulae are obtained for the sines of the phases
$S = 3/2$

$$\sin \delta_l = \frac{k}{4\pi} \cdot \frac{1}{2l+1} \cdot \left\{ \left(w + b + \frac{h+m}{2} \right) \int \varphi_l^{+} {}^* \, \overline{U} \, \psi'' \, d\tau - (h+m) \int \varphi_l^{+} {}^* \, U' \, \psi' \, d\tau \right\} \tag{27}$$

$S = 1/2$

$$\sin \delta_l = \frac{k}{4\pi} \cdot \frac{1}{2l+1} \cdot \frac{1}{\sqrt{2}} \left\{ \left(w + \frac{m}{2} - \frac{b-h}{2} \right) \int \varphi_l^{+} {}^* \, \overline{U} \, \psi'' d\tau - \left(w - m - \frac{b-h}{2} \right) \int \varphi_l^{+} {}^* \, \overline{U} \, \psi^s \, d\tau - (b - h + m) \int \varphi_l^{+} {}^* \, U' \, \psi' \, d\tau - (b+h) \int \varphi_l^{+} {}^* \, U' \, \psi^a \, d\tau \right\} \tag{27'}$$

Analogous formulae for the cosine of the phases are obtained starting from (24) and are omitted here for sake of brevity.

The above integral relations (27), (27)′ are very useful, because they permit the calculations of the phases for large energies of the impinging neutrons or whenever the phases are expected to be small. Furthermore, they yields a powerful device for checking the exactness of solutions obtained by approximate methods. One can also obtain with their help, as it will be apparent from a subsequent discussion, a fair general idea of the scattering, the latter depending mainly on the exchange properties of the interaction.

III. The variational method for the evaluation of the phases.

In view of the complexity of our problem, the best means of evaluating the phases at small energies as in the two body problem where the situation is far simpler, is offered by a variational method.

The usual variational principle which is based on the fact that the Hamiltonian is a Hermitian operator, and which has been successfully applied in the two body problem by L. Hulthen[3]), can be generalized for our problem in a quite natural way.

The fact of having put systematically into evidence the symmetry properties of the eigenfunctions and of the potentials brings about considerable simplifications in the calculations and makes a numerical calculation possible. The systems of equations (14), (15) can be rewritten in the form

$$\mathfrak{T} \, \psi_i = \sum\nolimits_\varkappa U_{i\varkappa} \, \psi_\varkappa$$

in which no distinction appears to existe between the two cases of $S = 3/2$ and $S = 1/2$. This means simply that for $S = 3/2$ one has

two ψ's, namely ψ' and ψ'' whereas for $S = 1/2$ there are four ψ's i. e. ψ^s, ψ^a, ψ', ψ''. $\mathfrak{T}$ is the symmetrical and Hermitian operator defined by (16) and $U_{i\varkappa}$ is a real and symmetrical matrix.
The integral

$$J = \Sigma_{i\varkappa} \int \psi_i^* \, (\delta_{i\varkappa} \mathfrak{T} - U_{i\varkappa}) \, \psi_\varkappa \, d\tau \qquad (28)$$

is stationary if ψ_i is a solution of the system (14) or (15) belonging to a given angular momentum and if the variations $\delta\psi_i$ vanish rapidly enough at $\varrho = \infty$ $q = \infty$, which implies that the varied functions have the same asymptotic behaviours. One has indeed

$$\delta J = \Sigma_{i\varkappa} \int \{ \delta\psi_i^* \, (\delta_{i\varkappa} \mathfrak{T} - U_{i\varkappa}) \, \psi_\varkappa + \psi_i^* \, (\delta_{i\varkappa} \mathfrak{T} - U_{i\varkappa}) \, \delta\psi_\varkappa \} \, d\tau$$

$$= \Sigma_{i\varkappa} \int \delta\psi_i^* \, (\delta_{i\varkappa} \mathfrak{T} - U_{i\varkappa}) \, \psi_\varkappa + \delta\psi_i \, (\delta_{i\varkappa} \mathfrak{T} - U_{i\varkappa}) \, \psi_\varkappa^* \} \, d\tau$$

and if the ψ's are solution of (14) or (15) i. e.

$$\mathfrak{T}\psi_i - \Sigma_\varkappa U_{i\varkappa} \psi_\varkappa = 0 \qquad\qquad \mathfrak{T}\psi_i^* - \Sigma_\varkappa U_{i\varkappa} \psi_\varkappa^* = 0$$

it follows that

$$\Sigma \delta\psi_i^* \, (\mathfrak{T}\psi_i - \Sigma_\varkappa U_{i\varkappa} \psi_\varkappa) = 0 \qquad \Sigma \delta\psi_i (\mathfrak{T}\psi_i^* - \Sigma_\varkappa U_{i\varkappa} \psi_\varkappa^*) = 0$$

hence

$$\delta J = 0$$

Conversely if $\delta J = 0$ for any variation $\delta\psi_i$ such that $(\delta\psi_i)_{q=\infty} = 0$ one has

$$\mathfrak{T}\psi_i = \Sigma U_{i\varkappa} \psi_\varkappa$$

Though ψ' and ψ'' are not independent functions it follows nevertheless from the relation

$$\int \{ \delta\psi'^* \, (\mathfrak{T}\psi' - \Sigma U \psi) + \delta\psi''^* \, (\mathfrak{T}\psi''^* - \Sigma U \psi) \} \, d\tau = 0$$

both that $\mathfrak{T}\psi' = \Sigma U \psi$ and that $\mathfrak{T}\psi'' = \Sigma U \psi$, because of the equality of the two integrals

$$\int \delta\psi'^* \, (\mathfrak{T}\psi' - \Sigma U \psi') \, d\tau = \int \delta\psi''^* \, (\mathfrak{T}\psi'' - \Sigma U \psi'') \, d\tau \qquad (29)$$

This equality follows immediately from the symmetry characteristics of the integrated functions.

Once a trial function is chosen for a particular angular momentum, the choice being such that it belongs to the correct symmetry class, has the right asymptotic behaviour, and depends from a certain number of variational parameters c_i besides the phase δ_l, one determines the constants c_i and δ_l by means of the equations

$$\left.\begin{aligned} J &= 0 \\ \frac{\partial J}{\partial c_i} &= 0 \end{aligned}\right\} \tag{30}$$

We can now write down explicitely the integrals to be made stationary. In the case $S = 3/2$ we can limit ourselves in view of the identity (29) to the integral

$$J^{(3/2)} = \int \psi_l''^* \{\mathfrak{T}\,\psi_l'' - (w+b)\,U^s\,\psi_l'' + (h+m)\,(U'\,\psi_l' - U''\,\psi_l'')\cdot\}\,d\tau \tag{31}$$

and for $S = 1/2$ to the integral:

$$\begin{aligned} J^{(1/2)} = &\int \psi^{a*}\{\mathfrak{T}\,\psi^a - (w+m)\,U^s\,\psi^a + 2\,(b+h)\,(U'\,\psi'' - U''\,\psi')\}\,d\tau \\ &+ \int \psi^{s*}\{\mathfrak{T}\,\psi^s - (w-m)\,U^s\,\psi^s - (b+h)\,(U'\,\psi' + U''\,\psi'')\}\,d\tau \\ &+ 2\int \psi''^*\{\mathfrak{T}\,\psi'' - (b-h)\,U''\,\psi^s + m\,(U'\,\psi' - U''\,\psi'') - w\,U^s\,\psi''\}\,d\tau \end{aligned} \tag{32}$$

We shall write also for $S = 3/2$ $\psi_l' = T'\cdot\psi_l$ and $\psi_l'' = T''\cdot\psi_l$ where ψ_l is a function symmetrical with respect to the permutation of 2 and 3. This way of writing is by no means restrictive; indeed for any two functions ψ', ψ'' which transform according to D one has

$$\begin{aligned} \psi' &= T'\cdot\left(-\frac{2}{3}\,\psi''\right) \\ \psi'' &= T''\cdot\left(-\frac{2}{3}\,\psi''\right) \end{aligned}$$

Conversely it is true, as we have mentioned earlier, that an arbitrary function symmetrical in the coordinates of 2 and 3 leads to a pair of functions which transform according to D, when acted upon by the operators T' and T''.

For the case $S = 3/2$, we can write $J^{(3/2)} = 0$ in the form

$$\int \psi_l''^*\,\Omega\,\psi_l\,d\tau = \left(w + b + \frac{h+m}{2}\right)\int U\,\psi_l''^*\,\psi_l\,d\tau - (h+m)\int U'\,\psi_l'^*\,\psi_l\cdot d\tau \tag{33}$$

To this purpose one has to observe that

$$2\,\psi_l'' = T^s\cdot\psi_l - 3\,\psi_l$$

that $T^s \cdot \psi_l$ is orthogonal to ψ_l'' and finally that the potential U_{23} has been split up. The symbols in (33) have the usual significance. In virtue of analogous considerations, we can write for $S = 1/2$, putting

$$\psi_l^s = T^s \psi_l \qquad \Phi_l' = T' \Phi_l \qquad \Phi_l'' = T'' \cdot \Phi_l$$

instead of

$$J^{(1/2)} = 0$$

the equality:

$$\int \psi_l^{s*} \Omega \psi_l d\tau - \int \Phi_l''^* \Omega \Phi_l d\tau + \frac{1}{3} \int \psi_l^{a*} \Omega \psi_l^a \cdot d\tau =$$
$$= \left(w - m - \frac{b-h}{2}\right) \int \psi_l^{s*} \overline{U} \psi_l d\tau - \left(w + \frac{m}{2} - \frac{b-h}{2}\right) \int \Phi_l''^* \overline{U} \Phi_l d\tau$$
$$+ (b - h + m) \cdot \int \Phi_l'^* U' \Phi_l d\tau + (b - h) \int (\psi_l - \Phi_l) [U''(\psi_l^s + \Phi_l''^*)$$
$$+ U' \Phi_l'^*] \cdot d\tau + \frac{1}{3} (w + m) \int U^s |\psi^a|^2 d\tau - \frac{2}{3} (b + h) \int (U' \psi_l'^*$$
$$- U'' \psi_l''^*) \psi_l^{a*} d\tau \qquad (33)'$$

IV. The interactions according to neutral and symmetrical theories.

We can use the integral relations (27) and (27)' derived for the phases to get a rigorous integral formula for the total cross-section To do this one has to use the well-known formula

$$f(\vartheta) = \sum_0^\infty {}_l (2l + 1) \frac{\sin \delta_l e^{i \delta_l}}{k} P_l(\cos \vartheta)$$

where $f(\vartheta)$ is the function which appears in (17) or (18).

Considering (22) one has

$$f(\vartheta) = \frac{1}{4\pi} \cdot \int e^{-i\vec{k}' \cdot \vec{q}} \varphi(r) \cdot \Omega \psi d\tau$$

$\Omega \psi$ is independent from the azimuthal angle about $\vec{k}$, $\vec{k}'$ is a vector of intensity k and forming an angle ϑ with $\vec{k}$. In view of (26) and (26)' one has finally

$$4\pi \cdot f^{(3/2)}(\vartheta) = \left(w + b + \frac{h+m}{2}\right) \int \varphi(r) e^{-i\vec{k}' \cdot \vec{q}} \overline{U} \psi'' d\tau - (h + m)$$
$$\cdot \int \varphi(r) \cdot e^{-i\vec{k}' \cdot \vec{q}} U' \psi' d\tau \qquad (34)$$
$$4\pi \cdot \sqrt{2} \cdot f^{(1/2)}(\vartheta) = \left(w + \frac{m}{2} - \frac{b-h}{2}\right) \int \varphi(r) e^{-i\vec{k}' \cdot \vec{q}} \overline{U} \psi'' d\tau$$
$$- \left(w - m - \frac{b-h}{2}\right) \int \varphi(r) e^{-i\vec{k}' \cdot \vec{q}} \overline{U} \psi^s d\tau$$
$$- (b - h + m) \int \varphi(r) e^{-i\vec{k}' \cdot \vec{q}} \overline{U}' \psi' d\tau + (b + h) \int \varphi(r) e^{-i\vec{k}' \cdot \vec{q}} U' \psi^a d\tau \quad (34')$$

These formulae become in the particular cases of a symmetrical or neutral interaction, as respectively given by (1) and (2).
Symmetrical theory

$$\left.\begin{aligned} f^{(3/2)}(\vartheta) &= -\frac{1}{4\pi}\cdot\frac{2}{3}\int \varphi(r)\, e^{-i\vec{k}'\cdot\vec{q}}\; U'\,\psi'\,d\tau \\ f^{(1/2)}(\vartheta) &= \frac{1}{4\pi}\cdot\frac{1}{\sqrt{2}}\cdot\left\{\frac{1}{2}\,g\cdot\int \varphi(r)\, e^{-i\vec{k}'\cdot\vec{q}}\; \overline{U}\,(\psi''+\psi^s)\,d\tau \right. \\ &\left. -\left(g-\frac{2}{3}\right)\int \varphi(r)\, e^{-i\vec{k}'\cdot\vec{q}}\,(\psi'-\psi^a)\; U'\,d\tau\right\} \end{aligned}\right\} \qquad (35)$$

Neutral theory

$$\left.\begin{aligned} f^{(3/2)}(\vartheta) &= -\frac{1}{4\pi}\int e^{-i\vec{k}'\cdot\vec{q}}\cdot\varphi(r)\;\overline{U}\,\psi''\,d\tau \\ f^{(1/2)}(\vartheta) &= \frac{1}{4\pi}\cdot\frac{1}{\sqrt{2}}\cdot\left\{\left(\frac{3}{2}\,g-1\right)\int \varphi(r)\, e^{-i\vec{k}'\cdot\vec{q}}\;\overline{U}\,(\psi''-\psi^s)\,d\tau \right. \\ &\left. +\,g\cdot\int \varphi(r)\, e^{-i\vec{k}'\cdot\vec{q}}\; U'\,(\psi'+\psi^a)\,d\tau\right. \end{aligned}\right\} \qquad (36)$$

It is a quite noteworty fact that for $S = 3/2$ the scattering by interactions of the symmetrical type results from the eigenfunction ψ' only, whereas with neutral interactions it comes from the eigenfunction ψ'' alone.

ψ' is antisymmetrical in the coordinates of the nucleons 2 and 3 and this implies necessarily an exchange of the impinging neutron with one of the nucleons of the initial deuteron. As a consequence of the conservation of momentum which is particularly apparent in the momentum space of $\vec{r}$ and $\vec{q}$, especially at high energies, the neutron will preferentially scattered backwards.

ψ'' is symmetrical in the coordinates of 2 and 3, reduces to the deuteron eigenfunction times a plane wave when the neutron 1 is at large distances from the deuteron 2, 3; in this case a scattering without exchange is also allowed, becoming preponderant at higher energies and giving an important contribution to forward scattering. For $S = 1/2$ one can follow an analogous argument. Assuming symmetrical theories, there is now a wave $\psi'' + \psi^s$ which appears in the first integral and vanishes rapidly at large distances from 1 to 2 and 3, by interference (Cfr. 18) whereas in the case of neutral theories there appears on the contrary a wave $\psi'' - \psi^s$ which obviously does not cancel out. This fact accounts again for a preferential scattering in the forward direction.

The eigenfunction ψ^a which is antisymmetrical in all three nuclear coordinates implies a strong polarisation of the initial deuteron and should be of importance at very low energies only. The variational formulae for calculating the phases individually (35) and (33)′ have a structure similar to that of the formulae just discussed, inasmuch as the same constants appear as factors of the various integrals, our arguments should have an even more general significance. It is owing to this feature that the N-D scattering becomes particularly interesting.

The formulae (27) and (27)′ for evaluating the phases read for the particular cases of symmetrical and neutral theories as follows
Symmetrical theory

$$S = 3/2 \qquad \sin \delta_l = -\frac{2}{3} \frac{k}{4\pi} \cdot \frac{1}{2l+1} \int \varphi_l^{+*} U' \psi_l' \cdot d\tau$$

$$S = 1/2 \qquad \sin \delta_l = -\frac{k}{4\pi} \frac{1}{2l+1} \cdot \int \varphi_l^{+*} \overline{U} \psi_l'' \, d\tau \tag{37}$$

Neutral theory

$$S = 3/2 \qquad \sin \delta_l = \frac{1}{\sqrt{2}} \cdot \frac{k}{4\pi} \cdot \frac{1}{2l+1} \cdot \left\{ \frac{1}{2} g \cdot \int \varphi_l^{+*} \overline{U} (\psi_l'' + \psi_l^s) \, d\tau - \left(g - \frac{2}{3}\right) \cdot \int \varphi_l^{+*} U' (\psi_l' - \psi_l^a) \, d\tau \right\}$$

$$S = 1/2 \qquad \sin \delta_l = \frac{1}{\sqrt{2}} \cdot \frac{k}{4\pi} \cdot \frac{1}{2l+1} \cdot \left\{ \left(\frac{3}{2} g - 1\right) \int \varphi_l^{+*} \overline{U} (\psi'' - \psi^s) \, d\tau + g \int \varphi_l^{+*} U' (\psi_l' + \psi_l^a) \, d\tau \right\} \tag{38}$$

V. Preliminary numerical calculations.

In analogy to the two-body problem the evaluation of the phases is quite simple if one can make use of the imperturbed solution in the formulae (37) and (38). This may be certainly be done for small phases. For small energies the phases corresponding to higher orbital momenta and for high energies all the phases are small. For neutrons of 2.5 MeV for istance the phase δ_1 can be calculated in this way without introducing an appreciable error.
Putting

$$\psi(r, q) = e^{i\vec{k} \cdot \vec{q}} \cdot \varphi(r)$$

one can write in this case for S = 3/2

$$\psi' = T' \cdot \psi; \qquad \psi'' = T'' \cdot \psi$$

and for $S = 1/2$

$$\psi^s = T^s \cdot \psi \qquad \psi' = T' \cdot \psi \qquad \psi'' = T'' \cdot \psi \qquad \psi^a = 0$$

Denoting by J_1, J_2, J_3 the integrals

$$J_1 = \int \varphi(r)\, e^{-i\vec{k}'\cdot\vec{q}}\, U_{13}\cdot\psi\, d\tau,$$

$$J_2 = \int \varphi(r)\, e^{-i\vec{k}'\cdot\vec{q}}\, U_{23}\cdot(23)\psi\, d\tau;\; J_3 = \int \varphi(r)\, e^{-i\vec{k}'\cdot\vec{q}}\, U_{13}\,(13)\psi\, d\tau$$

(37) and (38) can be written in the following form
Symmetrical theories

$$f^{(3/2)}(\vartheta) = \frac{1}{4\pi}(J_3 - J_2)$$

$$f^{(1/2)}(\vartheta) = \frac{1}{8\pi}\cdot(J_2 + (3g-1)\,J_3) \qquad (39)$$

Neutral theories*)

$$f^{(3/2)}(\vartheta) = \frac{1}{4\pi}\cdot(2\,J_1 - J_2 - J_3)$$

$$f^{(1/2)}(\vartheta) = \frac{1}{8\pi}\cdot(2\,(2-3\,g)\,J_1 + J_2 + (1-3\,g)\,J_3) \qquad (39)'$$

The integration to be carried out are straightforward if one chooses Gaussian functions both for the potentials and for the eigenfunction of the ground state of the deuteron, as has been already done by various authors[7])[8]).

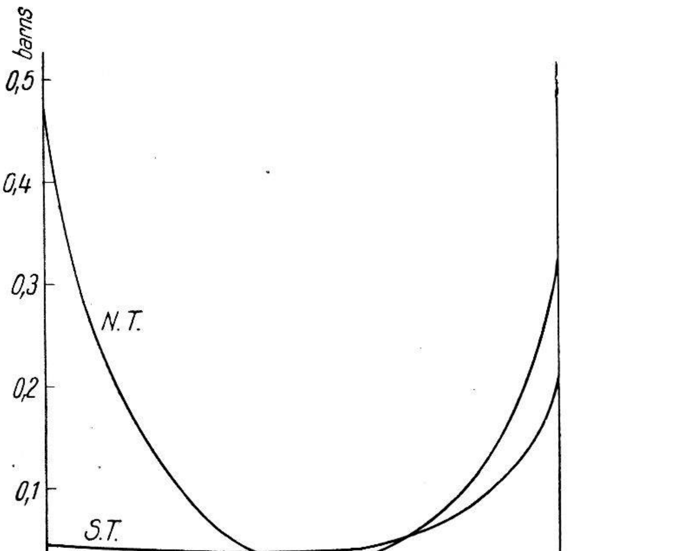

Fig. 1.

Angular dependence in the C. M. system of the scattering of 20 MeV neutrons by deuterons. The upper curve refers to neutral (N. T.) and the lower one to symmetrical theories (S. T.). The ordinates are in barns (10^{-24} cm^2). The total cross-section is 1.54 barns for N. T. and 0.71 barns for S.T.

*) These formulae have been given also by T. Y. Wu and J. Ashkin[7]). This ist not the case for the symmetrical theories, because these authors have failed to use rigorously the isotopic spin formalism.

For the case of neutrons of 20 MeV, where this approximation is expected to be a good one, the neutral and the symmetrical theories lead to the two curves shown in fig. 1.

The numerical constants which we have adopted are

$$\varkappa^{-1} = 1.9 \times 10^{-13} \text{ cm. (range of the forces)}$$

$$\varkappa^{-2}\, U_{23} = 5.22\, e^{-\varkappa^2 |r_3 - r_2|^2}$$

and this corresponds to a potential of 45 MeV for the deuteron in the ^3S state.

$$\varphi(r) = \left(\mu \sqrt{\frac{2}{\pi}}\right)^{3/2} e^{-\mu^2 r^2}$$

The constant $\mu^2 = 0.347\,\varkappa^2$ is determined by minimizing the energy of the deuteron in the ground state. With these values one has

$$\varkappa J_1 = 29.0\, e^{-0.74 k^2 (1 - \cos\vartheta)}; \qquad \varkappa J_2 = 58.0\, e^{-k^2 (1.45 + 1.16 \cos\vartheta)};$$
$$\varkappa J_3 = 24.2\, e^{-k^2 (0.49 + 0.0085 \cos\vartheta)}$$

A pronounced maximum only at 180^0 is a characteristic feature of the symmetrical theories and is also produced at smaller energies. Therefore the results of Buckingham and Massey[9]), who find for neutrons of 11.5 MeV a pronounced maximum only in the forward direction for symmetrical as well as for neutral theories, are hard to reconcile with the considerations made above.

Our curves have been calculated using values of g = 0.2 (N.T.) and g = 1.4 (S.T.) which accounts for the energy difference between the two S states of the deuteron, a ratio od 0.6 of the potential in the ^3S state to that in the ^1S state being assumed. On the other hand, in doing this one ignores the tensor force, which is predominantly responsible in the symmetrical theories for the difference between the ^3S and the ^1S levels.

Using g = 0.1 the angular dependence of the scatterins (S.T.) is still of the same type, but the total cross-section is lowered from 0.71 barns (corresponding to g = 1.4) to 0.2 barns.

In conclusion we wish to indicate in detail the formulae by which the phases can be evaluated using the variational method.

In the case $S = 3/2$, we may, putting

$$\psi_l = \varphi_l^+ G_l^+ \cos\delta_l + \varphi_l^- G_l^- \sin\delta_l$$

where ψ_l^+, φ_l^- are defined by (21), make use of the ansatz

$$\psi_l' = T' \cdot \psi; \qquad \psi_l'' = T'' \cdot \psi_l$$

The functions ψ_l' and ψ_l'' have the right symmetry character, belong to an angular momentum $l(l+1)\hbar$ and show an asymptotic behaviour as given by (17) .The trial functions G_l^+ and G_l^- must be chosen so as to approach unity rapidly when q goes to infinity. Furthermore q_l^- must also vanish rapidely enough for $q = 0$ to make ψ_l finite everywhere. The functions G contain the variational parameters which are determined by means of the equations (30).

For the actual calculation one must evaluate the following five integrals

$$J_1 = \int \psi_l^* U_{13} \psi_l \, d\tau \quad J_2 = \int \psi_l^* U_{13} (12) \psi_l \cdot d\tau, \quad J_3 = \int \psi_l^* U_{13} (13) \psi_l \, d\tau$$

$$J_4 = \int \psi_2^* \Omega \, \psi_l \, d\tau \qquad J_5 = \int [(12) \, \psi_l^*] \cdot \Omega \, \psi_l \, d\tau \tag{40}$$

It is useful to transform J_4 in the following manner. As one has

$$J_4 = \cos^2 \delta_l \cdot \int (\varphi_l^+ G_l^+)^* \, \Omega \, (\varphi_l^+ G_l^+) \cdot d\tau +$$
$$+ \frac{1}{2} \sin 2\, \delta_l \int [(\varphi_l^+ G_l^+)^* \, \Omega \, (\varphi_l^- G_l^-) + (\varphi_l^- G_l^-)^* \, \Omega \, (\varphi_l^+ G_l^+)] \cdot d\tau$$
$$+ \sin^2 \delta_l \cdot \int (\varphi_l^- G_l^-)^* \, \Omega \, (\varphi_l^- G_l^-) \, d\tau \tag{41}$$

and the identity

$$(\varphi_l^+ G_l^+)^* \, \Omega \, (\varphi_l^- G_l^-) -$$
$$(\varphi_l^- G_l^-) \, \Omega \, (\varphi_l^+ G_l^+) = (\varphi_l^+ G_l^+)^* \, (\Delta_r + \Delta_q) \, (\varphi_l^- G_l^-) -$$
$$(\varphi_l^- G_l^-)^* \, (\Delta_r + \Delta_q) \, (\varphi_l^+ G_l^+) = \mathrm{Div}_r \cdot [(\varphi_l^+ G_l^+)^* \cdot \nabla_r \, (\varphi_l^- G_l^-) -$$
$$(\varphi_l^- G_l^-)^* \, \nabla_r \, (\varphi_l^+ G_l^+)] + \mathrm{Div}_q [\varphi_l^+ G_l^+)^* \, \nabla_q \, (\varphi_l^- G_l^-) -$$
$$(\varphi_l^- G_l^-)^* \, \nabla_q \, (\varphi_l^+ G_l^+)]$$

one obtains integrating over all space, taking into account (20)

$$\int (\varphi_l^+ G_l^+)^* \, \Omega \, (\varphi_l^- G_l^-) \, d\tau = \int (\varphi_l^- G_l^-)^* \, \Omega \, (\varphi_l^+ G_l^+) \, d\tau - \frac{4\pi}{k} (2l+1).$$

The integral

$$\int (\varphi_l^- G_l^-)^* \, \Omega \, (\varphi_l^+ G_l^+) \, d\tau$$

can be written

$$\int (\varphi_l^- G_l^-)^* \Omega (\varphi_l^+ G_l^+) d\tau = \int (\varphi_l^- G_l^-)^* \varphi_l^+ (\Delta_r + \Delta_q) G_l^+ d\tau$$

$$+ 2 \int (\varphi_l^- G_l^-)^* \{\nabla_r \varphi_l^+ \nabla_r G_l^+ + \nabla_q \varphi_l^+ \nabla_q G_l^+ \} d\tau =$$

$$= \frac{4\pi}{k} (2l+1) \int_0^\infty G_l^{-*} \frac{\partial G_l^+}{\partial q} \cdot dq - 4\pi (2l+1) \int_0^\infty I_l^+ (kq) I_l^- (kq)$$

$$\cdot \left(\frac{\partial G_l^+}{\partial r} \cdot \frac{\partial G_l^{-*}}{\partial r} + \frac{\partial G_l^+}{\partial q} \cdot \frac{\partial G_l^{-*}}{\partial q} \right) q^2 dq$$

One obtains finally using in analogous way Green's theorem for the integrals which appear in (41) as factors of $\cos^2 \delta_l$ and $\sin^2 \delta_l$

$$J_4 = -\cos^2 \delta_l \int |\varphi_l^+|^2 [|\nabla_r G_l^+|^2 + |\nabla_r G_l^-|^2] d\tau$$

$$+ \frac{4\pi}{k} (2l+1) \sin 2\delta_l \cdot \left\{ \int_0^\infty G_l^{-*} \frac{\partial G_l^+}{\partial q} dq \right.$$

$$\left. - k \int_0^\infty I_l^+ I_l^- \left(\frac{\delta G_l^{+*}}{\partial r} \cdot \frac{\partial G_l^-}{\partial r} + \frac{\partial G_l^{+*}}{\partial q} \cdot \frac{\partial G_l^-}{\partial q} \right) q^2 dq - \frac{1}{2} \right\}$$

$$- \sin^2 \delta_l \cdot \int |\varphi_l^-|^2 [|\nabla_r G_l^-|^2 + |\nabla_r G_l^-|^2] \cdot d\tau \tag{42}$$

This form is more appropriate for numerical calculations. For the integral J_5 one can proceed in a similar manner and one finds

$$J_5 = \cos^2 \delta_l \cdot \int (\varphi_l^+ G_l^+)^* [(\Delta_r + \Delta_q) G_l^+ + 2 (\nabla_r \varphi_l^+ \cdot \nabla_r G_l^+$$

$$+ \nabla_q \varphi_l^+ \nabla_q G_l^+)] d\tau$$

$$+ \sin 2\delta_l \cdot \int (\varphi_l^- G_l^-)^* [(\Delta_r + \Delta_q) G_l^+ + 2 (\nabla_r \varphi_l^+ \nabla_r G_l^+$$

$$+ \nabla_q \varphi_l^+ \cdot \nabla_q G_l^+)] \cdot d\tau$$

$$+ \frac{1}{2} \sin 2\delta_l \int (\varphi_l^+ G_l^+)^* (U_{13} - U_{23}) (12) (\varphi_l^- G_l^-) d\tau$$

$$+ \sin^2 \delta_l \int (\varphi_l^- G_l^-)^* [(\Delta_r + \Delta_q) G_l^- + 2 (\nabla_r \varphi_l^- \cdot \nabla_r G_l^-$$

$$+ \nabla_q \varphi_l^- \cdot \nabla_q G_l^-)] d\tau \tag{43}$$

Equation (33) is written explicitely
Symmetrical theories

$$J_5 - J_4 + J_2 - J_3 = 0 \tag{44}$$

Neutral theories

$$J_5 - J_4 - 2\,J_1 + J_2 + J_3 = 0 \tag{44$'$}$$

Very great simplifications would result by choosing functions G_l independent of the coordinate r, i. e. disregarding the polarisation of the deuteron, and also using Gaussian potentials by taking for G linear combinations of Hermite functions. In the case $S = 1/2$ in the approximation where ψ is disregarded, we may put as above

$$\psi_l = \varphi_l^+ G_l^+ \cos\delta_l + \varphi_l^- G_l^- \sin\delta_l \qquad \psi_l^s = T^s \psi_l \qquad \psi_l^a = 0$$

$$\Phi_l = \varphi_l^+ Q_l^+ \cos\delta_l + \varphi_l^- Q_l^- \sin\delta_l \qquad \Phi' = T' \cdot \Phi_l \qquad \Phi'' = T'' \cdot \Phi_l$$

where the Q's can be of the same form as the G's but contain other variational parameters. The integrals are still the same ones, as in the case of $S = 3/2$, one has to add the integral

$$J_0 = \int \psi_l^* \, U_{23} \, \psi_l \, d\,\tau$$

The relation (33)$'$ may be written then in an explicit form as follows Symmetrical theories

$$\begin{aligned}(2\,J_5 - J_4)_{\psi,\psi} - (J_5 - J_4)_{\Phi,\Phi} &= -g\,(J_1 + J_2 + J_3)_{\psi,\psi} + g\,(J_1 + J_2 \\ &\quad - 2\,J_3)_{\Phi,\Phi} + (J_3 - J_2)_{\Phi,\Phi} \\ &\quad + \frac{1}{3}\,(g-2)\,\{(J_1 - J_2 + J_3 - J_0)_{\psi,\psi} + (J_1 - J_2 + J_3 - J_0)_{\Phi,\Phi} \\ &\quad - 2\,(J_1 + J_3 - J_0)_{\psi,\Phi} + 4\,\Phi\,(J_2)_{\psi,\Phi} - 2\,(J_2)_{\Phi,\psi}\}\end{aligned} \tag{45}$$

Neutral theories

$$\begin{aligned}(2\,J_5 - J_4)_{\psi,\psi} - (J_5 - J_4)_{\Phi,\Phi} &= (3\,g - 2)\,(J_1 + J_2 + J_3)_{\psi,\psi} + (3\,g - 2) \\ &\quad (J_1)_{\Phi,\Phi} - (3\,g - 1)\,(J_2)_{\Phi,\Phi} + (J_3)_{\Phi,\Phi} \\ &\quad - g\,\{(J_1 - J_2 + J_3 - J_0)_{\psi,\psi} + (J_1 - J_2 + J_3 - J_0)_{\Phi,\Phi} \\ &\quad - 2\,(J_1 + J_3 - J_0)_{\psi,\Phi} + 4\,(J_2)_{\psi,\Phi} - 2\,(J_2)_{\Phi,\psi}\}\end{aligned} \tag{45$'$}$$

The notation used is almost selfexplanatory, e. g.

$$(J_2)_{\psi,\Phi} = \int \psi_l^* \, U_{13}\,(12)\;\Phi_l \, d\,\tau$$

In a forthcoming paper we shall take up in great detail the actual evaluation of the integrals and of the phases δ_0 for smaller energies.

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