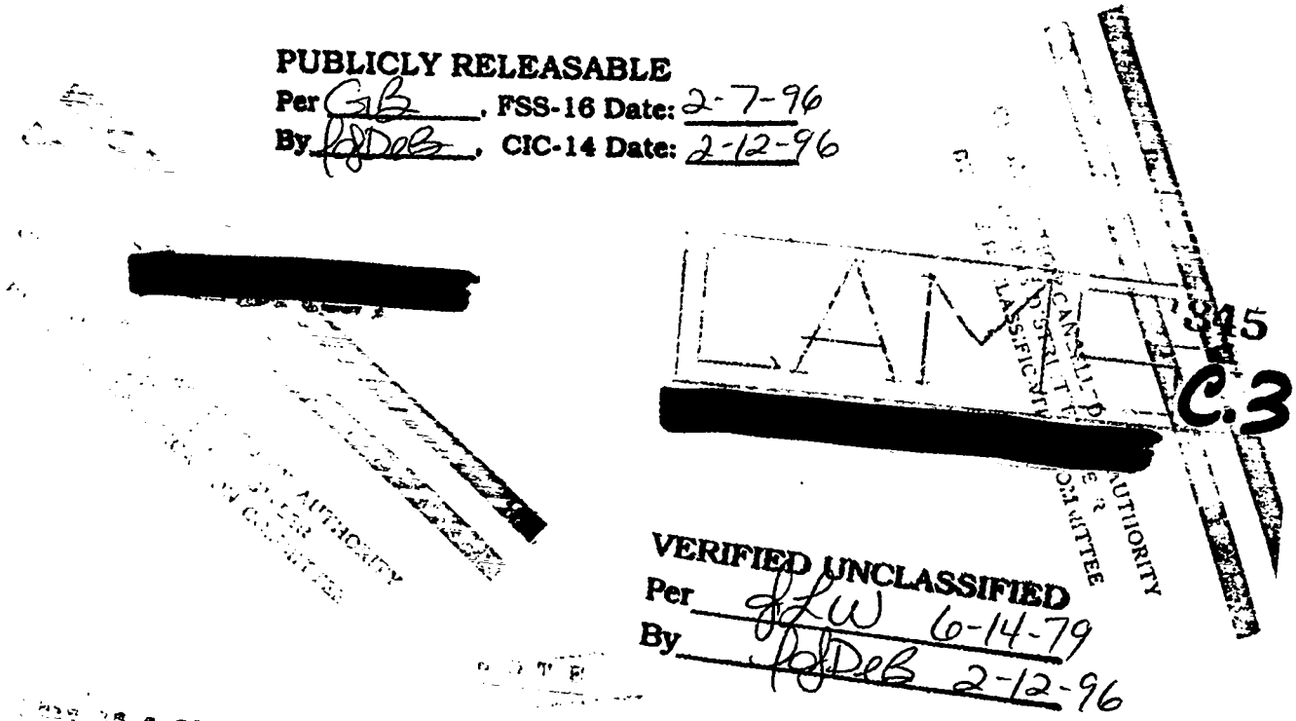
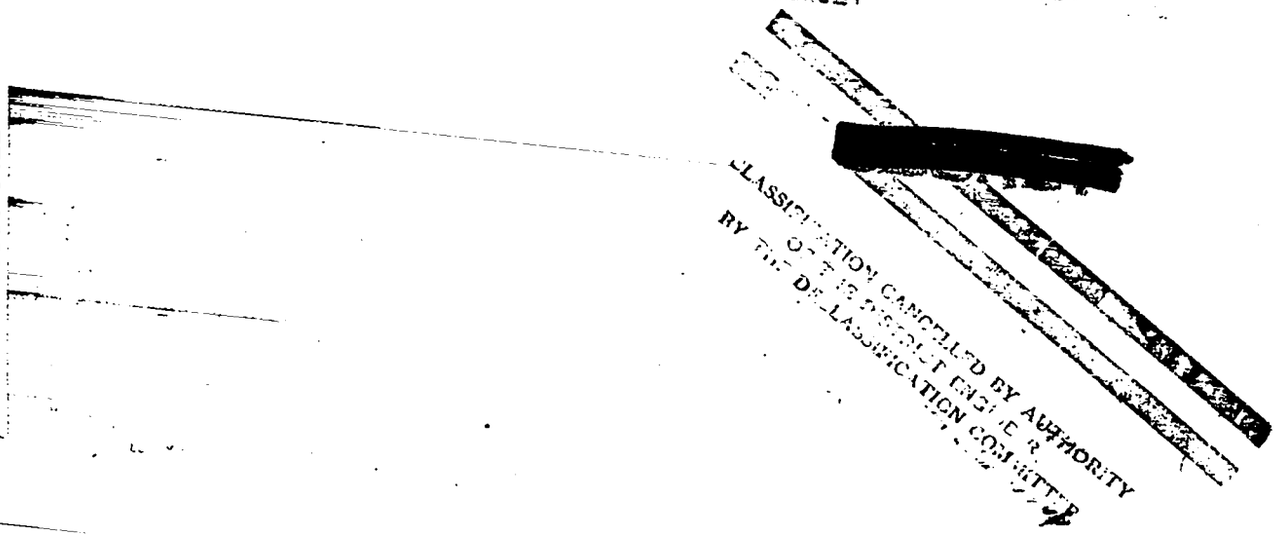


[illegible] is a cover sheet for a SECRET [illegible]
document must be [illegible] of this
left unattended or [illegible] must be
to it. When not in use [illegible] person may have access
safe. While this d[illegible] in a locked file or
have obtained a sig[illegible] until you
responsibility that the information contained [illegible] your
promised.

THE ENEMY WANTS THE INFORMATION CONTAINED IN THIS DOCUMENT.
DON'T LET HIM GET IT THROUGH YOUR NEGLIGENCE.



LAMS - 345

February 6, 1946

This document contains 10 pages

SPIN-DEPENDENT PART OF THE NEUTRON - DEUTERIUM CROSS SECTION

by
T. Hall
F. de Hoffmann

ABSTRACT

A matrix method for the spin-dependent part of the neutron-deuterium scattering cross section is worked out in detail. The method follows closely the treatment of Condon and Shortley for the evaluation of the dot product of matrices.

SPIN-DEPENDENT PART OF THE NEUTRON - DEUTERIUM CROSS SECTION

We wish to present a method for the spin-dependent part of the scattering cross section for slow neutrons from ortho and para deuterium. To introduce the problem let us quote from a forthcoming paper by Schwinger and Hammermesh[1]:

"We wish to calculate the differential cross section for a scattering process in which a neutron with momentum p^0 collides with a D_2 molecule with momentum $-p^0$ in the internal state specified by the vibrational, rotational and spin quantum numbers v, J, S, thereby producing a neutron with momentum p which has been scattered through the angle Θ into the solid angle $d\Omega$, leaving the molecule in the state characterized by $-p$, v', J', S'. The differential cross section, as computed by the Born approximation, is

$$\sigma_{J',v',S';\ J,v,S}(\Theta)d\Omega = \frac{16}{25}\frac{p}{p^0}\frac{1}{2(2S+1)(2J+1)}\sum_{m^1,m^1_J,m^1_S}\sum_{m_1\,m_J,m_S}\left|\left(\psi_f\,\frac{MV}{2\pi\hbar^2}\,U\psi_i\right)\right|^2 d\Omega \qquad (1)$$

which differs formally for the corresponding H_2 molecule cross section[2] only by the replacement of the numerical factor 4.9, the square of the reduced mass of the neutron - H_2 molecule system, by 16/25, the square of the reduced mass of the neutron - D_2 molecule system. These reduced mass factors arise

---

1). Schwinger and Hammermesh, the scattering of slow neutrons by ortho and deuterium. To be published in the Physical Review.

2). Schwinger and Teller, Phys Rev 52, 1937, 286-295 equation 21

in calculating the number of final neutron states per unit range of the total energy, and in the value of the neutron flux relative to the molecule."

Now we know that the interaction can be written as [3]

$$U = -\frac{2\pi\hbar^2}{M}\left[\left\{4a_{3/2} + 2a_{1/2}\right\} + 2(a_{3/2}-a_{1/2})\sigma_n\cdot(\sigma_1+\sigma_2)\right]\left[\delta(r_n-r_1) + \delta(r_n-r_2)\right]$$
$$-\frac{2\pi\hbar^2}{M}\left[2(a_{3/2}-a_{1/2})\,\sigma_n\cdot(\sigma_1-\sigma_2)\right]\left[(r_n-r_1) - (r_n-r_2)\right] \qquad (2)$$

where M is the mass of the neutron; $a_{3/2}$ and $a_{1/2}$ are the scattering amplitudes for a neutron - deuteron quadruplet interaction and a neutron - deuteron doublet interaction respectively; σ_1 and σ_2 are the spin vectors of the deuterons; σ_n is the spin vector of the neutron; r_1, r_2 and r_n are the respective position vectors and is the Dirac delta function. Units are such that the spin of the neutron is one half. The nature and use of these vectors is exactly as that given in Condon and Shortley "Theory of Atomic Spectra", Cambridge 1935 (hereafter referred to as C and S) and we follow their method in deriving the interaction matrices.

Let us set

$$\left.\begin{aligned}\alpha &= 4a_{3/2} + 2a_{1/2}\\ \beta &= 2(a_{3/2} - a_{1/2})\end{aligned}\right\} \qquad (3)$$

thus

$$U = -\frac{2\pi\hbar^2}{M}\left[\alpha + \beta\sigma_n\cdot(\sigma_1+\sigma_2)\right]\left[(r_n-r_1) + (r_n-r_2)\right]$$
$$-\frac{2\pi\hbar^2}{M}\left[\beta\sigma_n\cdot(\sigma_1+\sigma_2)\right]\left[\delta(r_n-r_1) - \delta(r_n-r_2)\right] \qquad (4)$$

3). One way of deriving this formula is given by Schwinger and Hammermesh and leads to their equation (6). The apparent difference is due to their definition of σ, in particular $\sigma_n = (1/2)\sigma_{\text{Schwinger}}$

We note that U is divided into a symmetrical and anti-symmetrical part and rewrite U as

$$U = U_1 \delta(+) + U_2 \delta(-) \tag{5}$$

Further we may rewrite the summation part of (1) using this symbolism as:

$$\sum_{m^1, m_J^1, m_S^1} \sum_{m_1 m_J m_S} \left| \psi_{\xi 2} \frac{MV}{2\pi\hbar^2} U \psi_i \right|^2 = A_1 B_1 + A_2 B_2 \tag{6}$$

where

$$\left.\begin{aligned} A_1 &= \sum_{m^1, m_S^1} \sum_{m, m_S} \left| (m_1 m_S \; U_1 \; m^1, m_S^1) \right|^2 \\ A_2 &= \text{same with } |U_2| \end{aligned}\right\} \tag{7}$$

and

$$\left.\begin{aligned} B_1 &= \sum_{m_J} \sum_{m, r_0} \left| \int \xi \delta(+) \}_i \; d\tau \right|^2 \\ B_2 &= \text{same with } \delta(-) \end{aligned}\right. \tag{8}$$

where and $_i$ are the final and initial spacial wave functions of the whole system and is their coordinate space.

In the following we wish to show the method for evaluating A_1 and A_2. Let us recall that

m = z component of neutron spin

m_J = z component of the rotation vector of the molecule

m_S = z component of $\sigma_1 + \sigma_2$

Our problem is essentially to obtain the elements of the matrices $\sigma_n \cdot (\sigma_1 + \sigma_2)$

and $\sigma_n \circ (\sigma_1 - \sigma_2)$. We shall perform this by evaluating $\sigma_n \circ \sigma_1$ first. The evaluation of $\sigma_n - \sigma_2$ is virtually the same problem. To get $\sigma_n \circ \sigma_1$ instead of summing over m and m_s, we change to a complete set of commuting variables $(J_1, J_2, J, J_z, \gamma)$ and sum over j, j_z where

$$J_1 = \sigma_1 + \sigma_2$$

$$J_2 = \sigma_n$$

$$J = \sigma_1 + \sigma_2 + \sigma_n$$

J_z = the z component of J

γ = the remaining variables completing the set

and small letters denote the eigenvalues of these variables. We note that our J_2 and σ_1 now satisfy the conditions for vectors P and Q as given by C and S page 70 where a scheme for the evaluation of P·Q is given.

The matrix elements of P∘Q are seen to be evaluated in terms of two quantities of the form $(\text{---} \vdots Q \vdots \text{---})$ and $(\text{---} \vdots P \vdots \text{---})$. The evaluation of these quantities in detail is given by equation C and S 10^3 2a and 10^3 2b. Their substitution into the evaluation of 12^3 2 then gives P∘Q.

For a given molecular spin S, the values of J, J_1 and J_2 will determine the role of the second deuteron spin so that we may apply the argument of C and S regarding relative phases (cf C and S, last paragraph of page 69) with the following results: for elements diagonal in j, j_1 and j_2 the value of $\sigma_n \circ \sigma_1$ and $\sigma_n \circ \sigma_2$ are the same; elements off the diagonal are the negative of each other. Therefore the diagonal elements of $\sigma_n \circ (\sigma_1 - \sigma_2)$ are zero and the off-diagonal elements of $\sigma_n \circ (\sigma_1 - \sigma_2)$ are zero.

This means that collisions in which the total molecular spin changes are due only to interaction terms of the form $\sigma_n \circ (\sigma_1 - \sigma_2)$ i.e. only due to U_2, the

[redacted]

antisymmetrical part of the interaction. Thus for the case in which total molecular spin changes $A_1 = 0$ and we need to evaluate only A_2. Similarly in those cases in which the total molecular spin remains unchanged $A_2 = 0$ and we need to evaluate only A_1.

The possible values of S for deuterium are 0, 1 and 2. Let us now treat the individual cases by the method outlined above.

I. SYMMETRIC

$A_2 = 0$ and

$$A_1 = \sum_{j,j_z} \sum_{j^1,j_z^1} \left| (j,j_z \left| a + \beta \sigma_n \cdot (\sigma_1+\sigma_2) \right| j^1,j_z^1) \right|^2 \qquad (9)$$

By our previous arguments regarding $\sigma_n \cdot (\sigma_1+\sigma_2)$ the matrix $a + \sigma_n \cdot (\sigma_1+\sigma_2)$ is diagonal (a being just a constant). Substitution into the formula for P.Q also shows that two elements with the same j and different j_z are equal. The summation over j_z therefore gives

$$A_1 = \sum_j (2j+1) \left\{ a+\beta\sigma_n \cdot (\sigma_1+\sigma_2) \right\}^2 \qquad (10)$$

In all symmetric cases $(\text{---} \vdots P \vdots \text{---}) = 1$ and $(\text{---} \vdots Q \vdots \text{---}) = 1/2$

Let us now look at all the possible symmetric cases in detail

Case I-1:

S goes from $0 \rightarrow 0$

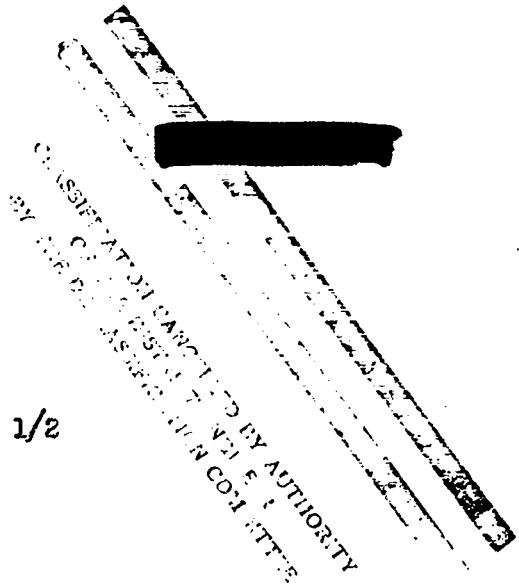
The only possible eigenvalues are

$$j = 1/2, \quad j_1 = 0, \quad j_2 = 1/2$$

Substitution of these values in P.Q gives $\sigma_n \cdot (\sigma_1+\sigma_2) = 0$

Hence

$$A_1 = 2a^2$$



Case I - 2:

S goes from 1 ⟶ 1

There are two possible sets of eigenvalues

$$j = 1/2, \quad j_1 = 1, \quad j_2 = 1/2$$

Here $\sigma_n \circ (\sigma_1 + \sigma_2) = 1$

or $j = 1\,1/2, \quad j_1 = 1, \quad j_2 = 1/2$

Here $\sigma_n \circ (\sigma_1 + \sigma_2) = 1/2$

Hence $$A_1 = 6\alpha^2 + 3\beta^2$$

Case I - 3

S goes from 2 ⟶ 2

There are two possible sets of eigenvalues

$$j = 1\ 1/2, \quad j_1 = 2, \quad j_2 = 1/2$$

Here $\sigma_n \circ (\sigma_1 + \sigma_2) = -3/2$

or $j = 2\ 1/2, \quad j_1 = 2, \quad j_2 = 1/2$

Here $\sigma_n \circ (\sigma_1 + \sigma_2) = 1$

Hence $$A_1 = 10\alpha^2 + 15\beta^2$$

[redacted]

[redacted]

II Anti-Symmetrical

By analagous arguments to the symmetrical case we obtain $A_1 = 0$ and

$$A_2 = \sum_j (2_j+1) \left\{ \beta \sigma_n \circ (\sigma_1 - \sigma_2) \right\}^2 \tag{11}$$

In all anty-symmetrical cases $(\longleftarrow \vdots P \vdots \longrightarrow)$ has the value 1/2 and $(\longleftarrow \vdots Q \vdots \longrightarrow)$ takes on different values as listed in each case.

Case II - 1

S goes from $0 \longrightarrow 1$

For this case $(\longleftarrow \vdots Q \vdots \longrightarrow) = \sqrt{2/3}$

There are two possible sets of eigenvalues

$$j = 1/2, \quad j_1 = 0 \longrightarrow 1, \quad j_2 = 1/2$$

Here $\sigma_n \circ (\sigma_1 - \sigma_2) = \sqrt{2}$

or $j = 1\ 1/2, \quad j_1 = 0 \longrightarrow 1, \quad j_2 = 1/2$

Here $\sigma_n \circ (\sigma_1 - \sigma_2) = 0$

Hence $A_2 = 4\beta^2$

Case II - 2

S goes from $1 \longrightarrow 0$

This is analagous to the $0 \longrightarrow 1$ case, and yields

$$A_2 = 4\beta^2$$

[redacted]

Case II - 3

S goes from $1 \rightarrow 2$

For this case $\left(\text{—}\vdots Q \vdots\text{—}\right) = \frac{1}{2\sqrt{3}}$

There are two possible sets of eigenvalues

$$j = 1\ 1/2, \quad j_1 = 1 \rightarrow 2, \quad j_2 = 1/2$$

Here $\sigma_n \cdot (\sigma_1 - \sigma_2) = \sqrt{15}$

or $$j = 2\ 1/2, \quad j_1 = 1 \rightarrow 2, \quad j_2 = 1/2$$

Here $\sigma_n \cdot (\sigma_1 - \sigma_2) = 0$

Hence

$$A_2 = 5\beta^2$$

The above method is interesting largely because it can be extended to other elements with relative ease.

The calculation of the hydrogen case is almost no extra work once the deuterium case is dealt with. If the interaction is written of the form of equation (4) where α and β simply have a different meaning then the values of A_1 and A_2 just evaluated change only because of a changed $\left(\text{—}\vdots P \vdots\text{—}\right)$ and $\left(\text{—}\vdots Q \vdots\text{—}\right)$ in the case of hydrogen.

We are contemplating the extension of this method to CH_4 and possibly NH_3.

[redacted]