LA-5196-MS

INFORMAL REPORT

Scattering Formulas for the Two-Particle Reaction

los alamos scientific laboratory

of the University of California

LOS ALAMOS, NEW MEXICO 87544

UNITED STATES
ATOMIC ENERGY COMMISSION
CONTRACT W-7405-ENG. 36

In the interest of prompt distribution, this LAMS report was not edited by the Technical Information staff.

Printed in the United States of America. Available from
National Technical Information Service
U. S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151
Price: Printed Copy $3.00; Microfiche $0.95

los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87544

LA-5196-MS
Informal Report
UC-32 & 34
ISSUED: February 1973

Scattering Formulas for the Two-Particle Reaction

by

C. J. Everett
E. D. Cashwell

SCATTERING FORMULAS
FOR THE TWO-PARTICLE REACTION

by

C. J. Everett and E. D. Cashwell

ABSTRACT

After a general (non-relativistic) treatment of transmutation resulting in two particles, the formulas obtained are specialized to give the laboratory energy-angle dependence for the inelastic (n,n´)-reaction and the elastic (n,n)-collision, in a form adapted to computation. These results are required for Monte Carlo neutron codes when the differential cross sections for such reactions are given in the laboratory frame, and in any case, for the "point detector" routine.

I. PARAMETERS OF A SYSTEM

Let S be a system of particles i, with velocities V_i, rest masses $m_i>0$, rest energies $e_i = m_ic^2$, momenta $P_i = m_iV_i$, and kinetic energies $k_i = \frac{1}{2} m_iV_i^2$; and with the totals

$$m_S = \sum m_i \quad e_S = \sum e_i \quad P_S = \sum P_i \quad k_S = \sum k_i \quad (1)$$

The velocity of its center of mass (CM) is then

$$V_S = \sum \frac{m_i}{m_S} V_i \quad (2)$$

whence $$m_SV_S = P_S \quad (3)$$

The velocities relative to the CM being

$$V_i' = V_i - V_S \quad (4)$$

it follows that

$$P_S' \equiv \sum m_iV_i' = 0 \quad k_S' \equiv \sum \frac{1}{2} m_iV_i'^2 = k_S - \frac{1}{2} m_SV_S^2 \quad (5)$$

From Fig. 1, one verifies the LAB/CM transformation

$$V_i^2 = V_S^2 + V_i'^2 + 2|V_S||V_i'|a_i' \; ; \; a_i' \equiv \cos \psi_i'$$

$$a_i = \{|V_S| + |V_i'|a_i'\}/|V_i| \; ; \; a_i \equiv \cos \psi_i$$

which may be written as

$$V_i^2/V_S^2 = (1+V_i'^2/V_S^2) + 2a_i'(|V_i'|/|V_S|) \quad (6)$$

$$a_i = (1+a_i'|V_i'|/|V_S|)/(|V_i|/|V_S|) \quad (7)$$

With the obvious identifications, these are of the form $X^2 = (1+B^2) + 2a_i'B$, $a_iX = 1 + a_i'B$, from which a_i' may be eliminated, with the result $X = a_i \pm \{a_i^2-(1-B^2)\}^{1/2}$, or explicitly

$$|V_i|/|V_S| = a_i \pm (a_i^2-K)^{1/2} \; ; \; K = 1-V_i'^2/V_S^2 < 1 \quad (8)$$

Note that, if $|V_i'|$ and $|V_S|$ are <u>prescribed</u> (as they may be when S results from a transmutation), there are the three possible cases of Fig. 2. Cases I, II, III are distinguished by the inequalities

$$|V_i'| \lesseqgtr |V_S| \quad \text{or} \quad 0 \lesseqgtr K \quad .$$

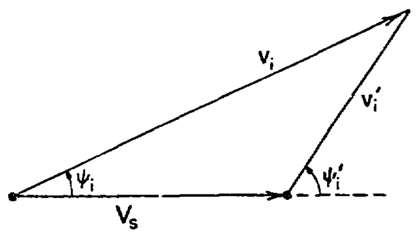

Fig. 1.

In Case I, it is apparent from the figure that the limiting LAB angle $\bar{\psi}_i$ has $\sin \bar{\psi}_i = |V_i'|/|V_S|$, or equivalently, $\bar{a}_i \equiv \cos \bar{\psi}_i = \sqrt{K}$. For a given LAB cosine $a_i = \cos \psi_i$, there are two possible LAB speeds $|V_i|$; and therefore it is clear that both signs (±) are required in (8).

In Case II, equations (6-8) take the simple form $V_i^2/V_S^2 = 2(1 + a_i')$, $a_i = \left|\frac{1}{2}(1 + a_i')\right|^{1/2}$, $|V_i|/|V_S| = 2a_i$. Note that $\cos \psi_i = \cos (\psi_i'/2)$, and $\psi_i = \psi_i'/2$, a relation obvious in Fig. 2. The limiting LAB angle is $\pi/2$.

In Case III, $|V_i|$ is again uniquely determined by a_i, which now ranges over the entire interval $[-1,1]$, and the (+) sign is mandatory in (8), since $K < 0$.

In terms of energy, equations (6-8) and their properties are summarized in the following:

$$k_i/k_i^* = 1 + (k_i'/k_i^*) + 2a_i'(k_i'/k_i^*)^{1/2} \quad ; \qquad k_i^* \equiv \frac{1}{2} m_i V_S^2 \tag{9}$$

$$a_i = \left|1 + a_i'(k_i'/k_i^*)^{1/2}\right| \Big/ (k_i/k_i^*)^{1/2} \tag{10}$$

$$k_i/k_i^* = \left|a_i \pm (a_i^2 - K)^{1/2}\right|^2 \; ; \; K = 1 - k_i'/k_i^* \tag{11}$$

Case I. $k_i' < k_i^*$; (±) in (11),

$$\bar{a}_i = \sqrt{K} \leq a_i \leq 1 \tag{12}$$

Case II. $k_i' = k_i^*$, $k_i/k_i^* = 2(1 + a_3')$

$$a_i = \left|\tfrac{1}{2}(1 + a_i')\right|^{1/2}, \; k_i/k_i^* = 4a_i^2 \, , \; 0 \leq a_i \leq 1 \, . \tag{13}$$

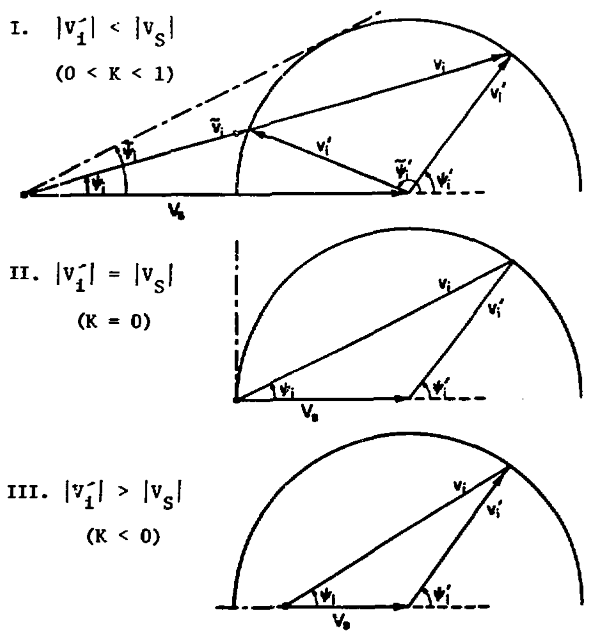

Fig. 2.

Case III. $k_i' > k_i^*$; (+) in (11), $-1 \leq a_i \leq 1$. (14)

If S consists of just two particles $i = 3, 4$, with <u>specified</u> m_3, m_4, k_S', then k_3', k_4' are uniquely determined in the (CM) frame by the equations $k_3' + k_4' = k_S'$, $P_3' + P_4' = 0$. For we then have

$$m_3 V_3'^2 + m_4 V_4'^2 = 2k_S' \qquad m_3^2 V_3'^2 - m_4^2 V_4'^2 = 0 \tag{15}$$

and consequently $m_S m_3 V_3'^2 = 2m_4 k_S'$, $m_S m_4 V_4'^2 = 2m_3 k_S'$, that is,

$$k_3' = \frac{m_4}{m_S} k_S' \qquad k_4' = \frac{m_3}{m_S} k_S' \tag{16}$$

II. TRANSMUTATION

A transmutation

$$A \to S$$

of such a general system A of particles h, into a second system S of particles i, is governed (in non-relativistic approximation) by the three conservation laws

$$m_A = m_S (\equiv m) \qquad P_A = P_S \qquad k_A + e_A = k_S + e_S \tag{17}$$

where the first ignores changes in total rest mass, and the third does not. The conservation of energy may be expressed in the form

$$k_A + Q = k_S \tag{18}$$

where $$Q \equiv e_A - e_S \tag{19}$$

is the "Q-value" of the reaction.

These laws, together with the relations (3), (5), for both A and S, imply that

$$V_A = V_S (\equiv V) \tag{20}$$

i.e., the CM velocity is unchanged, and hence the reaction in the common CM frame is governed by the laws

$$k_A' + Q = k_S' \qquad P_A' = 0 = P_S' \tag{21}$$

The first equation implies the necessary (and sufficient) condition

$$k_A' \geqslant (-Q) \tag{22}$$

for the transmutation to be mechanically possible.

If S is a two-particle system, its CM kinetic energies are necessarily those in (16), where $k_S' = k_A' + Q$ is determined by the system A and the e_i of S.

III. TWO-PARTICLE REACTIONS WITH "TARGET AT REST"

We consider here only the case of transmutations $A \to S$, where A consists of two particles $h = 1,2$, with the target 2 at rest ($V_2 = 0$), and S consists also of just two particles $i = 3,4$.

For the system A, we find from (2), (4) (since $V_2 = 0$)

$$V \equiv V_A = \frac{m_1}{m} V_1 \quad , \quad V_1' = \frac{m_2}{m} V_1 \quad , \quad V_2' = -\frac{m_1}{m} V_1 \quad ; \tag{23}$$

$m \equiv m_A$

and therefore

$$k_1' = \frac{m_2^2}{m^2} k_1 \qquad k_2' = \frac{m_1 m_2}{m^2} k_1 \qquad k_A' = \frac{m_2}{m} k_1 \tag{24}$$

The condition (22) now reads

$$k_1 \geqslant \frac{m}{m_2} (-Q) \equiv k_T \tag{25}$$

where $k_T \lesseqgtr 0$ is the (k.e.) threshold for the reaction. Since $k_1 > 0$, this is restrictive only when $Q < 0$, i.e., $e_A < e_S$. (We use k_T in general as a convenient parameter.)

Supposing the reaction possible, we find from (16,21,24) that the energy k_3' is uniquely determined as

$$k_3' = \frac{m_2 m_4}{m^2} k_1 (1 - k_T/k_1) \tag{26}$$

Moreover, the relation $V = \frac{m_1}{m} V_1$ of (23) implies

$$k_3^* \equiv \frac{1}{2} m_3 V^2 = \frac{m_1 m_3}{m^2} k_1 \tag{27}$$

Substitution of (26), (27) in (9-14) then yields, for $i = 3$, the following summary for the present reaction:

$$\frac{m^2}{m_1 m_3} (k_3/k_1) = \left(1 + \frac{m_2 m_4}{m_1 m_3}\right) - \frac{m_2 m_4}{m_1 m_3} (k_T/k_1) + 2a_3' \left\{\frac{m_2 m_4}{m_1 m_3} (1 - k_T/k_1)\right\}^{1/2} \; ; \; k_T = \frac{m}{m_2} (-Q) \lesseqgtr 0 \tag{28}$$

$$a_3 = \left\{1 + a_3' \left[\frac{m_2 m_4}{m_1 m_3} (1 - k_T/k_1)\right]^{1/2}\right\} \Bigg/ \left\{\frac{m^2}{m_1 m_3} (k_3/k_1)\right\}^{1/2} \tag{29}$$

$$\frac{m^2}{m_1 m_3}(k_3/k_1) = \left| a_3 \pm (a_3^2 - K)^{1/2} \right|^2 \quad ;$$

$$K = 1 - \frac{m_2 m_4}{m_1 m_3}(1 - k_T/k_1) = \frac{m m_4}{m_1 m_3}\left(\frac{-Q}{k_1}\right) - \frac{m(m_4 - m_1)}{m_1 m_3} \quad (30)$$

Case I. $k_1(m_4 - m_1) < m_4(-Q)$; ($\pm$) in (30),

$$\bar{a}_3 = \sqrt{K} \leq a_3 \leq 1 \quad (31)$$

Case II. $k_1(m_4 - m_1) = m_4(-Q)$; $a_3 = \left|\frac{1}{2}(1 + a_3')\right|^{1/2}$,

$$0 \leq a_3 \leq 1 \ , \ 2(1 + a_3') = \frac{m^2}{m_1 m_3}(k_3/k_1) \quad (32)$$

$$= 4a_3^2$$

Case III. $k_1(m_4 - m_1) > m_4(-Q)$; (+) in (30),

$$-1 \leq a_3 \leq 1. \quad (33)$$

In obtaining (30-33) we have used the definition $k_T = \frac{m}{m_2}(-Q)$, and the identity

$$m_2 m_4 - m_1 m_3 = m(m_4 - m_1).$$

We note here that whenever $m_4 > m_1$, the inequalities distinguishing the three cases may be written as

$$k_1 \lesseqgtr \frac{m_4}{m_4 - m_1}(-Q)$$

and if moreover $Q < 0$, then all three cases are possible, Case I obtaining in the incident energy interval

$$k_T = \frac{m}{m_2}(-Q) < k_1 < \frac{m_4}{m_4 - m_1}(-Q)$$

which is non-vacuous since $m(m_4 - m_1) = m_2 m_4 - m_1 m_3 < m_2 m_4$.

Again, if $m_4 > m_1$, and $Q \geq 0$, then necessarily $k_1 > 0 \geq \frac{m_4}{m_4 - m_1}(-Q)$, and Case III prevails.

IV. THE (n,n´) REACTION

We apply the foregoing results to an inelastic (n,n´) reaction, of form

$$n + \binom{A}{Z} \rightarrow n' + \binom{A}{Z}^*$$
$$1 \qquad 2 \qquad 3 \qquad 4$$

in which an incident neutron scatters from a nucleus at rest, leaving the latter in an excited state. In such a case, we assume

$$m_1 = m_3 < m_2 = m_4 \qquad Q = e_2 - e_4 < 0 \quad (34)$$

$-Q$ being the energy level excited. In terms of the usual parameter $A = m_2/m_1$, relations (28-33) reduce to

$$(A + 1)^2(k_3/k_1) = 1 + A^2 - A^2(k_T/k_1)$$
$$+ 2a_3'A(1 - k_T/k_1)^{1/2}; \ k_T = \frac{A+1}{A}(-Q) > 0 \ , \quad (35)$$
$$A = m_2/m_1 > 1$$

$$a_3 = \left|1 + a_3'A(1 - k_T/k_1)^{1/2}\right| / (A + 1)(k_3/k_1)^{1/2} \quad (36)$$

$$(A + 1)^2(k_3/k_1) = \left|a_3 \pm (a_3^2 - K)^{1/2}\right|^2 \ ;$$
$$K = A(A + 1)(-Q/k_1) - (A^2 - 1) \quad (37)$$

Case I. $k_T = \frac{A+1}{A}(-Q) < k_1 < \frac{A}{A-1}(-Q)$;

$$(\pm) \text{ in } (37),\ \bar{a}_3 = \sqrt{K} \leq a_3 \leq 1 \quad (38)$$

Case II. $k_1 = \frac{A}{A-1}(-Q)$, $a_3 = \left|\frac{1}{2}(1 + a_3')\right|^{1/2}$,

$$0 \leq a_3 \leq 1,\ 2(1 + a_3') = (A + 1)^2(k_3/k_1) \quad (39)$$
$$= 4a_3^2$$

Case III. $k_1 > \frac{A}{A - 1}(-Q)$; (+) in (37),

$$-1 \leqslant a_3 \leqslant 1. \qquad (40)$$

All three cases are possible, depending on the incident energy.

V. ELASTIC COLLISION

In an elastic collision

$$\underset{1}{n} + \underset{2}{\binom{A}{Z}} \to \underset{3}{n} + \underset{4}{\binom{A}{Z}}$$

one has

$$m_1 = m_3 \leqslant m_2 = m_4 \quad , \qquad Q = 0 = k_T \qquad (41)$$

and sees from (31-33) that Cases I, II, III are now distinguished by the inequalities

$$k_1(A - 1) \lesseqgtr 0 \quad ; \quad A \equiv m_2/m_1 \qquad (42)$$

Hence, for all nuclei but H, we have A > 1 and Case III prevails, formulas (28-30) being

$$(A + 1)^2(k_3/k_1) = 1 + A^2 + 2A\ a_3'; \ A = m_2/m_1 > 1 \ (43)$$

$$a_3 = \{1 + A\ a_3'\}/(A + 1)(k_3/k_1)^{1/2}; \ -1 \leqslant a_3 \leqslant 1 \ (44)$$

$$(A + 1)^2(k_3/k_1) = \left|a_3 + (a_3^2 - K)^{1/2}\right|^2 ; \qquad (45)$$

$$K = 1 - A^2 < 0.$$

Finally, for hydrogen (H) we assume A = 1, and see from (42) that Case II obtains for all incident energies k_1. The corresponding relations (32) then have the simple form

$$k_3/k_1 = \frac{1}{2}(1 + a_3') \ ; \ -1 \leqslant a_3' \leqslant 1 \qquad (A = 1) \qquad (46)$$

$$a_3 = \left|\frac{1}{2}(1 + a_3')\right|^{1/2} \quad ; \quad 0 \leqslant a_3 \leqslant 1 \qquad (47)$$

$$k_3/k_1 = a_3^2 \qquad (48)$$

As always in Case II, $\psi_3 = \psi_3'/2$ with $\frac{\pi}{2} > \psi_3 > 0$.

REFERENCES

1. E. D. Cashwell, C. J. Everett, A Practical Manual on the Monte Carlo Method (Pergamon Press, New York, 1959), Ch. V.
2. R. D. Evans, The Atomic Nucleus (Mc-Graw-Hill Book Co., Inc., New York, 1955), pp. 410-416.