INELASTIC SCATTERING OF NEUTRONS

I. QUASI-COMPound NUCLeUS THEORY

By W. K. Bertram*

[Manuscript received October 14, 1968]

Summary

The Feynman propagator formalism is used to derive a theory for the inelastic scattering of neutrons, in which the scattering amplitude contains direct and compound nucleus-like parts. The relation between this and the Feynman-diagram method of Shapiro is established.

Difficulties associated with the evaluation of the scattering amplitudes are discussed. In its present form the theory cannot be used to calculate cross sections owing to the large number of parameters in the expressions.

I. INTRODUCTION

There are two distinct theories to describe the scattering of neutrons by nuclei when the energy of the incident neutrons is sufficiently high for individual resonances not to be important \( E_n \gtrsim 1 \text{ MeV} \). For incident neutrons above approximately 10 MeV the direct reaction theory (e.g. Tobocman 1961) has been fairly successful. For neutron energies between 1 and 10 MeV, the compound nucleus theory of Hauser and Feshbach (1952) has been used.

The basic assumption of the compound nucleus theory is that the compound nucleus which is formed during the scattering process may be regarded as a real physical state so that the cross section for the reaction is the product of the cross sections for the formation and decay of the compound nucleus.

In this work we present a theory that incorporates features of both the direct reaction and the compound nucleus theories. The compound nucleus aspect of this theory differs from the conventional compound nucleus theory in that the intermediate nucleus no longer has any physical significance; in other words it is a virtual intermediate state and is therefore called a quasi-compound nucleus (QCN). The new theory also resembles the Feynman-diagram method of Shapiro (1961) which, however, lacks a sound theoretical foundation (Dar and Tobocman 1964).

The main disadvantage of the present theory is that, except perhaps for scattering of low energy neutrons by light nuclei, the amplitudes are difficult to evaluate owing to the presence of a large number of parameters. To make the theory useful it is necessary to find methods, probably based on statistical considerations, to reduce the number of parameters.

* Physics Division, Australian Atomic Energy Commission, Research Establishment, Private Mail Bag, Sutherland, N.S.W. 2232.

II. Propagators and the S-matrix

Suppose the Hamiltonian of a system is $H$ and the time-dependent wavefunction is $\Psi(x,t)$ such that

$$\left(-i\frac{\partial}{\partial t} + H\right)\Psi(x,t) = 0, \quad (1)$$

then the wavefunction at time $t = t_2$ can be related to the wavefunction at time $t = t_1 (t_1 < t_2)$ by the relation

$$\Psi(x_2,t_2) = \int K_+(x_2,t_2;x_1,t_1) \Psi(x_1,t_1) \, dx_1 \, dt_1. \quad (2a)$$

The kernel $K_+(x_2,t_2;x_1,t_1)$, which is defined by (2a), is known as the propagator of the system (Feynman 1948, 1949; Feynman and Hibbs 1965).

It is convenient to introduce the notation

$$(x_1,t_1) \rightarrow 1, \quad x_1 \rightarrow \hat{1},$$

so that (2a) now reads

$$\Psi(2) = \int K_+(2;1) \Psi(1) \, d1. \quad (2b)$$

The propagator $K_+$ satisfies the equation

$$\left(-i\frac{\partial}{\partial t_2} + H(2)\right)K_+(2;1) = \delta(2;1). \quad (3)$$

In particular, when $H(2)$ is the single-particle kinetic energy operator $T(2)$, the propagator is denoted by $K^0_+(2;1)$ and has the form

$$K^0_+(2;1) = \frac{-2Mi}{(2\pi)^4} \int \frac{\exp\{i(\mathbf{p} \cdot \mathbf{r}_{21} - Et_{21})\}}{p^2 - 2ME - i\epsilon} \, dp \, dE, \quad (4a)$$

where $M$ is the mass of the particle, $\mathbf{r}_{21} = \mathbf{r}_2 - \mathbf{r}_1$, and $t_{21} = t_2 - t_1$. It is obvious from (4a) that $K^0_+(2;1) = 0$ when $t_2 < t_1$. We may also define a propagator $K_-(2;1)$ which is nonzero for $t_2 < t_1$; then

$$K^0_-(2;1) = \frac{2Mi}{(2\pi)^4} \int \frac{\exp\{i(\mathbf{p} \cdot \mathbf{r}_{21} - Et_{21})\}}{p^2 - 2ME + i\epsilon} \, dp \, dE. \quad (4b)$$

We now omit the plus or minus suffix from the kernel and assume it to be plus when $t_2 > t_1$ and minus when $t_2 < t_1$.

When a particle has internal structure, i.e. when its Hamiltonian is of the form

$$H = H_1 + T,$$

where $H_1$ is the Hamiltonian for the internal motion of the particle, the propagator becomes

$$K(2;1) = \sum_{\nu} \phi_{\nu}(\hat{2}) \phi_{\nu}^*(\hat{1}) \exp\{-iE_\nu(t_2 - t_1)\}K^0(2;1), \quad (5)$$

where $K^0(2;1)$ is the free-particle propagator (4) for the motion of the centre of mass
of the particle, and $\phi_v$ are the eigenfunctions of $H_1$

$$H_1 \phi_v = E_v \phi_v. \quad (6)$$

If we separate the Hamiltonian of a system into two parts

$$H = H_0 + V,$$

where $V$ is usually some interaction between the various members of the system, the differential equation (3) may be expressed as the integral equation

$$K(2; 1) = K^0(2; 1) - i \int K^0(2; 3) V(3) K(3; 1) \, d3, \quad (7a)$$
or, equivalently,

$$K(2; 1) = K^0(2; 1) - i \int K(2; 3) V(3) K^0(3; 1) \, d3, \quad (7b)$$

where $K^0$ satisfies

$$\left( -i \frac{\partial}{\partial t} + H_0 \right) K^0(2; 1) = \delta(2; 1). \quad (8)$$

Assuming that as $t \to \pm \infty$ the particles of the system are sufficiently far removed from each other then, asymptotically,

$$H \to H_0.$$

If in the remote past, $t = t_1$, the system was in an eigenstate $\chi_i$ of $H_0$ then the amplitude for finding the system in an eigenstate $\chi_l$ in the distant future, $t = t_2$, is

$$S_{tl} = \int \chi_l^*(\hat{2}) K(2; 1) \chi_l(\hat{1}) \, d(\hat{1}, \hat{2}). \quad (9)$$

The matrix $S$, whose elements are $S_{tl}$, is just the $S$-matrix (Eckstein 1956; Brenig and Haag 1959; Newton 1966).

The transition matrix $T$, defined by the relation

$$S_{tl} = \delta_{tl} + (2\pi)^4 i T_{tl}, \quad (10)$$
is related to the scattering amplitude $M_{tl}$ by

$$T_{tl} = M_{tl} \delta(K_l - K_t) \delta(E_l - E_t), \quad (11)$$

where $K_l$, $E_l$, $K_t$, and $E_t$ are the total momenta and energies of the system in the incident and exit channels respectively.

When the scattering process under consideration is of the type

$$A + x \to A' + x', $$

the differential cross section in the centre-of-mass frame is

$$\frac{d\sigma}{d\Omega} = (2J_A + 1)^{-1} (2J_x + 1)^{-1} \frac{M_{Az} M_{A'x'} k_x' k_x}{(2\pi)^2} \left| M_{tl} \right|^2, \quad (12)$$

where it is assumed that the incident particles are not polarized, and

$$M_{Az} = M_A M_x / (M_A + M_x).$$
III. INELASTIC SCATTERING

Consider the inelastic scattering process

$$A + n \to A' + n', \quad (13)$$

where $A$ is a nucleus consisting of several nucleons and $n$ is a neutron. The Hamiltonian of this system can be written as

$$H = T_A + T_n + H_A + V, \quad (14)$$

where $T_A$ and $T_n$ are the kinetic energy operators for $A$ and $n$, $H_A$ is the Hamiltonian for the motion of the nucleons within $A$, and $V$ describes the interaction between $A$ and $n$.

Combining equations (7a) and (7b) the propagator for this system can be written in the form

$$K(2; 1) = K^0(2; 1) - i \int K^0(2; 3) V(3) K^0(2; 1) \, d3$$

$$\quad \quad - \int K^0(2; 3) V(3) K(3; 4) V(4) K^0(4; 1) \, d3,4. \quad (15)$$

Initially $A$ is assumed to be in an eigenstate $\phi_1$ (usually the ground state) of $H_A$, and after the reaction in some eigenstate $\phi_f$, such that in the construction of the $S$-matrix, the functions $\chi_l$ and $\chi_f$ are given as

$$\chi_l = \phi_l(x') \exp(iK_l \cdot r^A) \exp(iK_l \cdot r^n), \quad \chi_f^* = \phi_f^*(x') \exp(-iK_f \cdot r^A) \exp(-iK_f \cdot r^n). \quad (16)$$

Substituting (15) and (16) in (9) we see that the first term on the right of (15) yields $\delta_{1f}$, and thus from (10) the transition matrix is

$$T_{1f} = \frac{1}{(2\pi)^4} \int \chi_f^*(\hat{2}) K^0(2; 3) V(3) K^0(3; 1) \chi_l(\hat{1}) \, d(\hat{1}, \hat{2}, 3)$$

$$\quad \quad - \frac{i}{(2\pi)^4} \int \chi_f^*(\hat{2}) K^0(2; 3) V(3) K(3; 4) V(4) K^0(4; 1) \chi_l(\hat{1}) \, d(\hat{1}, \hat{2}, 3, 4).$$

From the definition of the propagators $K^0$ it follows that

$$\chi_f^*(3) = \int \chi_f^*(\hat{2}) K^0(2; 3) \, d\hat{2}, \quad \chi_l(3) = \int K^0(3; 1) \chi_l(\hat{1}) \, d\hat{1}, \quad (17)$$

and therefore the transition matrix can be written in the form

$$T_{1f} = -(2\pi)^{-4} \left( \int \chi_f^*(3) V(3) \chi_l(3) \, d3 - i \int \chi_f^*(3) V(3) K(3; 4) V(4) \chi_l(4) \, d(3, 4) \right). \quad (18)$$

The first term on the right of (18) is just the first Born approximation and can for example be calculated using a single-particle excitation model. It represents the direct reaction contribution to the scattering amplitude. The second term, which is of more importance at low neutron energies, contains compound nucleus-like contributions.
IV. QUASI-COMPOUND NUCLEUS TERM

The second term on the right of (18) can be evaluated using $\chi_1$ and $\chi_2$ as given by (16) and using the form (5) for the propagator $K(3; 4)$.

$$T_{11} = \frac{2MB}{(2\pi)^3} \int \phi_t^*(x_5) \exp[-i(K_1 \cdot r_5 + k_1 \cdot r_5^n - (E_1^A + E_1^n - \varepsilon_i^A)\ell_5)]$$

$$\times V(x_5, r_5^n) \sum \frac{\Psi_v^*(X_5)\Psi_v^*(X_6) \exp[i(P_B \cdot r_5^n - (E_B - \varepsilon_v^B)\ell_5)]}{P_B^2 - 2MBE_B - i\varepsilon}$$

$$\times \phi_1(x_6) \, d(5, 6) \, dP_B \, dE_B,$$

where $-\varepsilon_i^A (\varepsilon_i^A > 0)$ denotes the binding energy of $A$.

The functions $\Psi_v$, which are eigenfunctions of the total Hamiltonian (14), can be expanded in terms of the eigenfunctions $\phi_s$ of $H_A$ as

$$\Psi_v(X) = \sum \psi_{vs}(r^{An}) \phi_s(x),$$

where $\psi_{vs}$ satisfies the equation

$$\left(\frac{1}{2} M_n^{-1} \nabla^2 - (\varepsilon_v^B - \varepsilon_s^B)\right)\psi_{vs}(r) = \sum \psi_{st}(r) V_{st}(r),$$

with

$$M_{nA} = M_n M_A/(M_n + M_A),$$

and $V_{st}(r)$ is defined as

$$V_{st}(r) = \int \phi_s^*(x) \, V(x, r) \, \phi_t(x) \, dx.$$

If we change the variables of integration to $r = r^{An}$ and $R = r^B$, then the integrations over $t_5$, $t_6$, $E_B$, $R_5$, $R_6$, and $P_B$ can be seen to yield $\delta$-functions expressing conservation of energy and momentum. Therefore (19) becomes

$$T_{11} = 2MB \sum \left(\int \sum \psi_{vs}(r) \, V_{tt}(r) \exp(iq_2 \cdot r) \, dr\right)$$

$$\times \left((K_1 + k_1)^2 - 2MBE_B - i\varepsilon\right)^{-1} \left(\int \sum \psi_{vs}(r) \, V_{st}(r) \exp(-iq_1 \cdot r) \, dr\right)$$

$$\times \delta(E_{in} - E_{out}) \delta(K_{in} - K_{out}),$$

where

$$q_1 = (M_n/M_B)K_1 - (M_A/M_B)k_1, \quad q_2 = (M_n/M_B)K_1 - (M_A/M_B)k_1.$$

The potentials $V_{tt}$ and $V_{st}$ can be eliminated by using (22) and the relation

$$\int \nabla^2 \phi(r) \exp(ip \cdot r) \, dr = -p^2 \int \phi(r) \exp(ip \cdot r) \, dr.$$
Thus the scattering amplitude is

\[ M_{\text{ff}} = - \sum_{\nu(\text{bound})} \left( \int \psi_{\nu}(r) \exp(iq_{2}.r) \, dr \right) \left( \frac{1}{2} M_{nA}^{-1} q_{1}^{2} + (\vec{\sigma}_{v} - \vec{\sigma}_{s}) \right) \]

\[ \times \left( \int \psi_{\nu}(r) \exp(-iQ_{1}.r) \, dr \right) + 2M_{B} \sum_{\nu(\text{unbound})} (\ldots) . \]  

(26)

The summation over \( \nu(\text{bound}) \) is to be taken only over those terms containing \( \psi_{\nu} \) and \( \psi_{\nu}^{*} \) for which the eigenfunctions \( \Psi_{\nu} \) correspond to bound states. The summation over \( \nu(\text{unbound}) \) contains all the terms that correspond to unbound states of \( B \). The reason for this separation is that the relation (25) is valid only if \( \psi(r) \to 0 \) as \( r \to \infty \); it can therefore not be applied to unbound states.

The contributions to the scattering due to terms in (23) that correspond to unbound \( \Psi' \)'s contain the higher order scattering terms of the Born expansion. They are probably important if one wished to describe resonance phenomena. However, as the evaluation of these terms presents even greater difficulties than the evaluation of the bound state terms, we shall assume that they can be neglected, even though this assumption is very difficult to justify.

It may be worth noting that (26) can also be obtained using the time-independent Green's function or the Green's operator formalism (see e.g. Wu and Ohmura 1962).

V. INCLUSION OF INTRINSIC SPIN

So far we have completely ignored the intrinsic spins of the particles involved in the reaction. The introduction of spin is in this case fairly straightforward. Suppose the spins of \( A \) before and after the reaction are \( J_{A} \) and \( J'_{A} \) with corresponding \( z \) components of \( M_{A} \) and \( M'_{A} \). The scattering amplitude may now be evaluated as before. However, in this case the wavefunctions \( \phi_{n}(x) \) (see equations (16)), which previously were the wavefunctions for the internal motion of \( A \), are now assumed to include also the spin wavefunctions of both \( A \) and \( n \).

The expression of the wavefunction \( \Psi_{\nu}(X) \) in terms of \( \phi_{n} \) (equation (20)) is then

\[ \Psi_{\nu}(X) = \sum_{s,l,m,J} \langle J_{A}, M_{A}, \frac{1}{2}, \mu_{n} | J, M_{A} + \mu_{n} \rangle \langle J, M_{A} + \mu_{n}, l, m | J_{B}, M_{A} + \mu_{n} + m \rangle \]

\[ \times \psi_{\nu}^{lmJ}(r^{nA}) \phi_{n}(x) , \]  

(27)

where \( J \) is the channel spin and \( J_{B} \) is the spin of the intermediate particle \( B \). The summation over \( s \) does of course imply summation over \( J_{A}, M_{A} \), and \( \mu_{n} \), since \( \phi_{n}(x) \) contains these spin wavefunctions. The equation satisfied by \( \psi_{\nu}^{lmJ} \) is found to be

\[ \sum_{lmJ} \langle J_{A}, M_{A}, \frac{1}{2}, \mu_{n} | J, M_{A} + \mu_{n} \rangle \langle J, M_{A} + \mu_{n}, l, m | J_{B}, M_{A} + \mu_{n} + m \rangle \]

\[ \times \left\{ \frac{1}{2} M_{nA}^{-1} \nabla^{2} - (\vec{\sigma}_{v} - \vec{\sigma}_{s}) \right\} \psi_{\nu}^{lmJ} \]

\[ = \sum_{lmJ'} \langle J'_{A}, M'_{A}, \frac{1}{2}, \mu_{n}' | J', M'_{A} + \mu_{n}' \rangle \langle J', M'_{A} + \mu_{n}', l, m | J_{B}, M'_{A} + \mu_{n}' + m \rangle \]

\[ \times \psi_{\nu}^{lmJ}(r) V_{sd}(r) . \]  

(28)
Writing
\[ \psi_{ijs}^{lmj}(r) = G_{ijs}^{lj}(r) Y_{lm}(r), \]  
and using the expansion
\[ \exp(iq \cdot r) = 4\pi \sum_{L=0}^{\infty} \sum_{m=-L}^{L} \hat{j}_L(qr) Y_{Lm}(r) Y_{Lm}^*(q), \]
the scattering amplitude becomes
\[ M_{f1} = (4\pi)^{3/2} \sum_{J', M_A', \mu_n'} J_{i_{12}} \sum_{J, M_A, \mu_n} <J, M_A, \frac{1}{2}, \mu_n | J, M_A + \mu_n> \langle J, M_A + \mu_n, l_1, 0 | J_B, M_A + \mu_n> \]
\[ \times <J', M_A' + \mu_n', l_2, m | J_B, M_A + \mu_n> \]
\[ \times \left( \frac{1}{2} M_{nA}^{-1} q_1^2 + (\frac{\epsilon^B}{\epsilon}) - (\frac{\epsilon^A}{\epsilon}) \right) \left( \int G_{i1j}^{ij}(r) j_{i_1j}(q_1 r) r^2 dr \right) \]
\[ \times \left( \int G_{ij}^{i'j'}(r) j_{i_2j'}(q_2 r) r^2 dr \right) Y_{l_2m}(Q). \]  

We have taken the z axis along the direction of the incoming beam so that \( Q \) is the momentum transfer vector, \( Q = k_1 - k_f \), and, if we assume that the potential \( V(x, r) \) is spherically symmetric,
\[ \sum_J <J, M_A, \frac{1}{2}, \mu_n | J, M_A + \mu_n> \langle J, M_A + \mu_n, l, m | J_B, M_B> \]
\[ \times \left( \frac{1}{2} M_{nA}^{-1} \frac{d}{dr} \left( \frac{2}{r} \frac{d}{dr} \right) - \frac{l(l+1)}{r^2} \right) G_{ijs}^{lj} \]
\[ = \sum_{J', M_A', \mu_n'} <J', M_A', \frac{1}{2}, \mu_n' | J', M_A' + \mu_n'> \langle J', M_A' + \mu_n', l, m | J_B, M_B> \]
\[ \times G_{ij}^{i'j'}(r) V_{st}(r). \]  

VI. Connection with Feynman-Diagram Method

In the centre-of-mass frame, \( q_1 = k_1 \) and \( q_2 = k_f \).

Then
\[ E_1 = \frac{1}{2} M_{nA}^{-1} q_1^2 \]
is the total kinetic energy of the particles in the incident channel and
\[ E_f = \frac{1}{2} M_{nA}^{-1} q_2^2 \]
is the kinetic energy in the exit channel.
The amplitude $M_{fi}$ has a series of poles in the complex $E_i$ plane lying on the negative part of the real $E_i$ axis. To see this we note that if in (28) the potentials $V_{st}$ approach zero faster than $r^{-1}$ as $r \to \infty$, then asymptotically

$$G^{ij}_{vs}(r) \to N^{ij}_{vs} \kappa_{vs} h_i(\kappa_{vs} r),$$

(33)

where $h_i(z)$ is the spherical Hankel function of the first kind, $N^{ij}_{vs}$ is a complex constant closely related to the reduced width (Dullemond and Schnitzer 1963), and

$$\kappa_{vs} = 2M_{nA}(\delta^B_v - \delta^A_A).$$

(34)

The integrals in (31) therefore give rise to a factor $(q_1^2 + \kappa_{v1}^2)^{-1}(q_2^2 + \kappa_{v2}^2)^{-1}$, but

$$q_1^2 + \kappa_{v1}^2 = 2M_{nA}(E_1 + \delta^B_v - \delta^A_1), \quad \text{and} \quad q_2^2 + \kappa_{v2}^2 = 2M_{nA}(E_1 + \delta^B_v - \delta^A_1).$$

Also, from conservation of energy it follows that

$$E_1 + \delta^B_v - \delta^A_1 = E_1 + \delta^B_v - \delta^A_1.$$

Thus the amplitude has poles at

$$E_1 = -(\delta^B_v - \delta^A_1).$$

(35)

In fact (31) is identical with the amplitude corresponding to the sum of pole graphs (Fig. 1) of the dispersion theory of nuclear reactions (Shapiro 1961), this process being known as the quasi-compound nucleus process (Schnitzer 1965).

The summation extends over all internal states of $B$. In the dispersion theory of nuclear reactions the amplitude corresponding to a single pole graph is

$$M_{fi} = \Gamma_{v1}(q_1) \Gamma^*_v(q_1)/[(\frac{1}{2}M_{nA}q_1^2 + (\delta^B_A - \delta^A_1))],$$

(36)

where $\Gamma_{v1}$ and $\Gamma_{vt}$ are the vertex parts corresponding to the vertices 1 and 2 respectively,

$$\Gamma_{ vm}(q) = \left(\frac{1}{2}M_{nA}q^2 + (\delta^B_v - \delta^A_m)\right) \int G_{vm}^l(r) j_i(qr) r^2 dr,$$

(37)

and the denominator is the propagator for the motion of $B$ from 1 to 2.

We have, for the sake of simplicity, omitted the angular momentum and spin quantum numbers from (36) and (37). When these are included (see e.g. Shapiro and Timashev 1965) it is easily verified that, after the summations over all internal states of $B$ have been performed, the amplitude given by (36) is identical to (31).

It is important to note that we have derived (31) directly from Schrödinger's equation, whereas the Feynman-diagram method of dispersion theory lacks a sound theoretical basis in that it cannot be related to the many-body Schrödinger equation. It is instead based on a number of assumptions that are difficult to justify (Dar and Tobocman 1964).
VII. Evaluation of Amplitude

The main disadvantage of the theory is that the amplitude (31) is very difficult to evaluate numerically. Difficulties arise in the determination of the functions $G_{vl}$ and $G_{vt}$ which are solutions of the set of coupled differential equations (32). It is possible to replace (32) by a set of uncoupled single-particle equations by introducing suitably parameterized "optical" potentials $V_n^J(r)$ such that $G_{vn}^{IJ}$ is a solution of

\[
\left\{ \frac{1}{2M_{nA}} \frac{1}{r} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) - \frac{l(l+1)}{r^2} - V_n^J(r) - (\delta^B_v - \delta^A_n) \right\} G_{vn}^{IJ}(r) = 0. \tag{38}
\]

The functions $G_{vn}^{IJ}$ are then single-particle wavefunctions. They are not normalized but are subject to the condition

\[
\int \psi_v^* \psi_w \, dX = \delta_{vw}.
\]

$G_{vn}^{IJ}$ may also contain a phase factor that can only be determined by solving the original differential equations (32).

For scattering by heavy target nuclei certain assumptions about the statistical nature of the nuclei involved can be made in order to determine the functions $G_{vl}$ and thus make it possible to use (31) for the calculation of scattering cross sections. These assumptions and various other approximations are discussed in the following paper (present issue, pp. 145–53).

VIII. References


SHAPIRO, I. S. (1961).—Nucl. Phys. 28, 244.


