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Study of Deuteron Stripping Reaction by Coupled Channel Theory. I

——*Variational Formulation and Discussion on Basic Equations*——

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Close coupling equations for the rearrangement reaction $A+d\to B+p$ are derived from a variational principle for reaction amplitude assuming the usual stripping mechanism. The sum of the wave functions of the deuteron and proton channels is used as a trial function. An exact and simple expression for the error introduced into the reaction amplitude is also derived by applying the theory of finite variations. Our variational principle is not affected by the existence of ambiguity in defining the proton and deuteron wave functions of relative motion, which should be carefully considered for rearrangement reaction because of the "non-orthogonality" or channels. The origin of this non-uniqueness and the induced ambiguity in the optical potentials are discussed in connection with the relation between the present method and the method of the projection operators. The interaction kernel consists of two parts, one coming from the usual $V_{np}+V_{pA}-U_{pB}$ term and the other due to the non-orthogonality of the initial and final channel wave functions. It is shown that DWBA is obtained only if the whole interaction kernel (not $V_{np}+V_{pA}-U_{pB}$ alone) is considered as perturbation. The relation between the present method and the methods of projection operators is discussed.

§ 1. Introduction

The theory of direct reaction by means of distorted wave Born approximation (DWBA)[1] has become a powerful tool for analyzing the experimental data and extracting useful information concerning the nuclear structure through rather precise fitting of the theoretical predictions to the experimental observations.

In contrast to the success in the practical applications, it should be recognized that the theoretical basis of DWBA has not yet been fully established in general and the applicability of DWBA is judged still to a large extent by the fit of the theoretical predictions to the experimental data in each particular case. For inelastic scattering leading to collective excited states, however, a rather far reaching studies have been made by the method of coupled channels.[2),3)] Since this method takes account of the transition matrix elements between the strongly

coupled channels up to infinite order, DWBA may be regarded as an approximation corresponding to the weak coupling limit of this method. Thus, one can discuss the accuracy of DWBA by comparing the calculated results of DWBA with the "exact" calculation obtained by the coupled channels method.

For the (p, p') reaction leading to the first $2+$ vibrational states of medium weight nuclei it was found[4] that with the same distorting potential and coupling constant the cross section calculated by DWBA overestimates the cross section, for large values of the deformation parameter β being proportional to β^2 while the "exact" cross section is linear in β for $\beta>0.2$. It was found, however, for some cases that if the distorting potential in DWBA is readjusted so that it gives the same elastic cross section as the "exact" calculation, the cross section for inelastic scattering also agrees with the "exact" one.

The study of the theoretical basis of DWBA for rearrangement reactions is far less adequate. There are several factors peculiar to the rearrangement reactions which have to be born in mind. First, there are arguments[5] that the Born series for rearrangement collision diverges. Divergence of the Born series does not necessarily mean that the first order Born approximation, including DWBA, is inaccurate. None the less, it would be an unfavorable factor to be reckoned with in establishing the validity of DWBA. At least there would be no inherent error criterion in DWBA. The divergence stems from the presence of bound states both in the initial and in the final state such as deuteron and the bound neutron in the (d, p) reaction. For the inelastic scattering, therefore, Born series converges at least at high energies. Secondly, in the rearrangement reaction the wave functions in the initial and final channels are not orthogonal to each other. The non-orthogonality gives rise to a coupling term of the two channels whose nature has not yet been clarified. The third factor which is peculiar to the rearrangement reaction has been revealed in the calculation of electron pick-up from an atom by an incident proton. In the first order Born approximation the cross section of this process was shown to be proportional to E^{-6} at high energies. It was found, however, that if one goes one step further one finds a term proportional to $E^{-11/2}$ in the second Born approximation.[6] This implies that the first order term is surpassed by the second order term at high energies which is quite contrary to usual expectation.[7]

Several attempts have been made to construct a formalism of direct reaction theory which includes DWBA as a special case. The mathematically most rigorous one is probably the exact three-body problem approach[8] to the rearrangement process. In the (d, p) reaction, for instance, the process is regarded as a rearrangement of three particles, proton, neutron and the target nucleus which is assumed to be a structureless massive particle providing neutron with a binding potential. It has been shown that this problem is reduced to the solution of an equation with one independent variable and is practically soluble if one assumes a special, somewhat unrealistic form of the interaction, such as a zero range

potential, separable potential, etc.

Another method is to apply the method of coupled channels to rearrangement reactions. This method will simplify the comparison with Born approximation and will enable one to use realistic nucleon-nucleon, nucleon-nucleus and deuteron-nucleus interactions.

In atomic physics a calculation has been carried out for the elastic scattering of positron from hydrogen atom[9] by this method in which the closed channel of positronium formation is coupled to the elastic channel. A calculation is also being planned for the same process when the positronium channel is open.[10]

In nuclear physics, a method of coupled channels for rearrangement process has been formulated by Wheeler[11] in his resonating group theory*) which has been used for the analysis of few nucleon problems.[12]

The coupled-channel method has been applied to rearrangement reactions with heavier nuclei for the (γ, p), (d, d) and (t, p) reactions in which the p- and n channels,[13] d- and p channels[14] and t- and p channels[15] are coupled, respectively. In particular, Rawitscher[14] has carried out such a calculation for deuteron induced reaction on Ca^{40}, and found that the (d, d) cross section can be reproduced by a deuteron optical potential with a large imaginary part since the reduction of the deuteron wave function in the nuclear interior is recovered by the coupling with the stripping channel at the nuclear surface. This reduction, however, affects the (d, p) cross section in a way similar to a cutoff in DWBA, as Stamp suggested in (t, p) reactions.[15] In those applications to heavier nuclei the interaction which causes the transition is assumed to have zero range and the non-orthogonality terms are neglected.

Questions now arise as to what the main effects of the coupling of channels will be and under what condition the effect will be large. In considering these questions there are several factors which one immediately notices. In the (d, p) reaction, for instance, the size of the matrix element of the transition will depend on the neutron separation energy: if it is large the matrix element will be small, which might make one expect that DWBA is valid. Polological argument[16] suggests, however, that the opposite might be true since the smaller the neutron separation energy, the nearer the pole corresponding to DWBA approachs the physical region. Therefore, there is no off-hand criterion related to the neutron separation energy. The effect of channel coupling is expected to be larger for lower partial waves since the amplitudes of the lower partial waves are large in the neighbourhood of the nucleus. For the similar reason the giant resonance in the distorted wave may enhance the coupling and affect the reliability of DWBA. DWBA reproduces in general the angular distribution of stripping reactions well but there are many examples in which cutoff in the radial integral is needed to reproduce the observed maxima and minima.[17] Should this feature be really

*) The Rayleigh Ritz method used by Wheeler is, in principle, applicable to only bound state problems.

attributed to the channel coupling as asserted by Stamp[15] and Rawitscher?[14]

In this series of papers we investigate the method of coupled channels for nuclear rearrangement collisions, especially the (d, p) reaction, in which the initial and final channels are coupled together. From the observed fact that the stripping process has a large cross section one sees that these two channels are strongly coupled to each other. There may, however, be other channels which are also strongly coupled directly or indirectly to those channels.[2),18] In that case the coupling of all these channels should in principle be treated on equal footing. However, we shall content ourselves here by assuming that the effects of the channels other than the initial and final channels are somehow approximately taken into account by assuming a suitable phenomenological effective Hamiltonian with adjustable parameters. A criterion for the validity of such an assumption has been given by Buck and Rook[19] using the unitarity of S-matrix. We may use this criterion as one of the measures of reliability of our calculations. We should emphasize, however, that the truncation of other channels by the procedure described above is primarily for the sake of computational convenience. Even in such a restricted model, however, we hope to obtain some information about the effects of the coupling between the channels.

The method of coupled channels for inelastic scattering has been developed by expanding the total wave function in the complete set of intrinsic wave functions of the target nucleus and those of the projectile. In the case of rearrangement collision, however, this procedure is difficult to follow since the residual nucleus is different from the target nucleus, so that one has to deal with the wave functions of the initial and final channels which are not "orthogonal" to each other.

Under these circumstances, one of the best ways to derive the basic equations of the coupled-channel method for rearrangement collisions is probably to use a variational method, because the "best" wave functions of relative motion is obtained within the assumed form of the trial functions: the sum of the wave functions in the strongly coupled channels.

We derive in § 2 the basic equations of the present formalism for the (d, p) reaction from a variational principle by using the method of finite variation. Assuming that the target nucleus has no spin and neglecting the intrinsic spin of nucleons for simplicity, the basic equations are derived in the three-dimentional form in § 2.1 and in the form analyzed in partial waves in § 2.2. An expression for the error in the calculated S-matrix is also derived. In § 2.3 the formulae for the cross sections are given. In § 3 ambiguities in the wave functions and the effective Hamiltonian are discussed together with the relation between the present method and the method of projection operators.[24)~26] In § 4 the reaction amplitudes which arise from the non-orthogonality of channels and the relation of DWBA to the present method in the limit of weak coupling are discussed in detail. In § 5 a summary is given.

§ 2. Derivation of the basic coupled equations by the theory of finite variation

In this section, we first treat a simplified problem by the method of infinitesimal variation of Kohn's type.[23] Then, we derive the basic coupled equation by means of the method of finite variation. By the latter procedure one can obtain a simple and exact expression for the error in the calculated scattering matrix elements. The theory of finite variation has been developed by Kato[24] for scattering by a central potential. The theory in the subsequent subsections is a direct extension of that theory to rearrangement collisions. In order to avoid unnecessary complexities we neglect intrinsic spin of nucleons. We also assume that the target nucleus has no spin and that the D-state of deuteron can be neglected.

Let us denote the wave functions of the target nucleus, A, and the incident deuteron, d, by $\Phi_{00}^{A}(\xi)$ and $\phi_d(r_{np})$ respectively and also denote the wave function of the residual nucleus, B, by $\Phi_{l_n m_n}^{B}(\xi, \boldsymbol{r}_n)$ where l_n and m_n are the orbital angular momentum and its z-component of the captured neutron relative to the centre of mass of A. As shown in Fig. 1, $\boldsymbol{r}_{np}$ and $\boldsymbol{r}_n$ represent the relative coordinates between the proton and the neutron and between the neutron and A respectively. ξ stands for the aggregate of the intrinsic coordinates of A. The relative coordinates of the initial and final channels are denoted by $\boldsymbol{R}$ and $\boldsymbol{r}$ respectively.

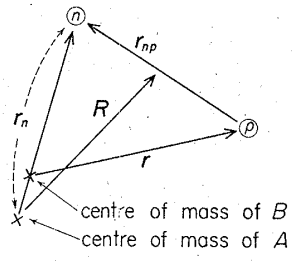

Fig. 1. Coordinate system for the reaction $A(d, p)B$.

The total Hamiltonian of the system, H, can be written in two alternative forms corresponding to the initial and final channels, respectively, as

$$H = H_A - a_{np}\Delta_{np}|_R + V_{np}(r_{np}) - a_d\Delta_R|_{np} + V_{nA}(r_n) + V_{pA}(r_p') \qquad (2\cdot1)$$

$$= H_B - a_p\Delta_r|_n + V_{pA}(r_p') + V_{np}(r_{np}), \qquad (2\cdot2)$$

where $\boldsymbol{r}_p'$ is the proton coordinate relative to the centre of mass of A and

$$H_B = H_A - a_n\Delta_n|_r + V_{nA}(r_n), \qquad (2\cdot3)$$

where the a's are given in terms of the reduced mass, μ, of the corresponding relative motion by $a = \hbar^2/(2\mu)$. In terms of the nucleon mass m_0 and the mass number A of the target nucleus, they are given by

$$a_{np} = \frac{\hbar^2}{m_0}, \quad a_d = \frac{A+2}{4A}\frac{\hbar^2}{m_0}, \quad a_p = \frac{A+2}{2(A+1)}\frac{\hbar^2}{m_0} \text{ and } a_n = \frac{A+1}{2A}\frac{\hbar^2}{m_0} \qquad (2\cdot4)$$

in the approximation that the binding energies of d, A and B are neglected. In (2·1) through (2·3) $\Delta_{np}|_R$ represents the Laplacian with respect to the variable

$\boldsymbol{r}_{np}$ when $\boldsymbol{R}$ is kept constant, when these two variables are taken as independent variables of the system. Similarly, $\Delta_R|_{np}$, $\Delta_r|_n$ and $\Delta_n|_r$ stand for the Laplacian with respect to $\boldsymbol{R}$, $\boldsymbol{r}$ and $\boldsymbol{r}_n$ respectively when $\boldsymbol{r}_{np}$, $\boldsymbol{r}_n$ and $\boldsymbol{r}$ are respectively kept constant. It is assumed that the interaction between the proton (neutron) and the target nucleus can be represented by a spherically symmetric potential V_{pA} (V_{nA}). If these potentials depend on ξ, reaction can proceed to a final state which is forbidden in the ordinary stripping and pick-up reaction mechanisms. We assume that this possibility can be neglected.

Now, the total wave function satisfies the Schrödinger equation

$$(H-E)\Psi=0\,, \tag{2·5}$$

and the normalized wave functions Φ^A_{00}, $\Phi^B_{l_nm_n}$ and ϕ_d satisfy the equations

$$H_A\Phi^A_{00}=E_A\Phi^A_{00}\,, \qquad H_B\Phi^B_{l_nm_n}=E_B\Phi^B_{l_nm_n}\,, \tag{2·6}$$

$$\{-a_{np}\Delta_{np}+V_{np}(r_{np})\}\,\phi_d(r_{np})=\varepsilon_d\phi_d(r_{np})\,, \tag{2·7}$$

respectively. We assume that

$$\Phi^B_{l_nm_n}=\Phi^A_{00}\phi_{l_nm_n}\,, \tag{2·8}$$

where $\phi_{l_nm_n}$ is defined by

$$\phi_{l_nm_n}(\boldsymbol{r}_n)=\int d\xi\Phi^{A*}_{00}(\xi)\,\Phi^B_{l_nm_n}(\xi,\,\boldsymbol{r}_n)\,, \tag{2·9}$$

and satisfies the equation,

$$\{-a_n\Delta_n+V_{nA}(r_n)\}\,\phi_{l_nm_n}(\boldsymbol{r}_n)=E_n\phi_{l_nm_n}(\boldsymbol{r}_n)\,. \tag{2·10}$$

The wave numbers k_d and k_p in the d and the p channel, respectively, are determined by

$$E=E_A+\varepsilon_d+E_d=E_B+E_p\,, \qquad E_d=a_dk_d^2, \qquad E_p=a_pk_p^2, \tag{2·11}$$

and the Q-value of the reaction is determined by

$$Q=E_A+\varepsilon_d-E_B=a_n\kappa^2-a_{np}\gamma^2, \tag{2·12}$$

where $i\kappa$ and $i\gamma$ are the imaginary wave numbers of the captured neutron and that of the internal motion of the deuteron, respectively. The functions Φ^A_{00}, $\Phi^B_{l_nm_n}$, ϕ_d and $\phi_{l_nm_n}$ are all assumed to be known and are not subject to variations in the following discussions.

2.1 *Derivation of the basic equations for the special case with* $l_n=0$

In this subsection we illustrate the general spirit of the present formalism by considering a simple special case in which the Coulomb potentials are absent and l_n is equal to zero.

Let us consider two special solutions of Eq. (2·5), $\Psi^{(1)}$ and $\Psi^{(2)}$, which satisfy, respectively, the following sets of boundary condition:

$$\Psi^{(1)}=\Phi^A\phi_d\chi_d^{(1)}(\boldsymbol{R})+\Phi^B\chi_p^{(1)}(\boldsymbol{r})+\psi^{(1)}, \tag{2·13}$$

where $\chi_d^{(1)}$ and $\chi_p^{(1)}$ have the asymptotic forms

$$\chi_d^{(1)}(\boldsymbol{R})\sim\exp(ik_d\boldsymbol{n}^{(1)}\boldsymbol{R})+\frac{f^{(1)}(\boldsymbol{n}^{(1)},\boldsymbol{n})}{R}\exp(ik_dR) \tag{2·13a}$$

and

$$\chi_p^{(1)}(\boldsymbol{r})\sim\frac{g^{(1)}(\boldsymbol{n}^{(1)},\boldsymbol{n}')}{r}\exp(ik_pr), \tag{2·13b}$$

respectively and $\psi^{(1)}$ vanishes asymptotically in the d- and p-channels and has only outgoing waves in the asymptotic region of all the other open channels, and

$$\Psi^{(2)}=\Phi^A\phi_d\chi_d^{(2)}(\boldsymbol{R})+\Phi^B\chi_p^{(2)}(\boldsymbol{r})+\psi^{(2)}, \tag{2·14}$$

where the asymptotic forms of $\chi_d^{(2)}$ and $\chi_p^{(2)}$ are given by

$$\chi_d^{(2)}(\boldsymbol{R})\sim\left(\frac{g^{(2)}(\boldsymbol{n}^{(2)},\boldsymbol{n})}{R}\exp(ik_dR)\right)^* \tag{2·14a}$$

and

$$\chi_p^{(2)}(\boldsymbol{r})\sim\left(\exp(ik_p\boldsymbol{n}^{(2)}\boldsymbol{r})+\frac{f^{(2)}(\boldsymbol{n}^{(2)},\boldsymbol{n}')}{r}\exp(ik_pr)\right)^*, \tag{2·14b}$$

respectively and $\psi^{(2)}$ satisfies the same boundary condition as $\psi^{(1)}$, except that the former has only incoming waves in the asymptotic region. In the above equations the subscripts for Φ^A and Φ^B representing the angular momenta are dropped, and unit vectors $\boldsymbol{n}\equiv\boldsymbol{R}/R$, $\boldsymbol{n}'\equiv\boldsymbol{r}/r$ and $\boldsymbol{n}^{(i)}$ ($i=1$ and 2) are used. $\Psi^{(1)}$ represents an ordinary scattering state in which the deuteron is incident on the target nucleus A in the direction $\boldsymbol{n}^{(1)}$. $\Psi^{(2)}$, on the other hand, represents the time reversed wave function of the state in which the proton is incident on the residual nucleus B in the direction of $\boldsymbol{n}^{(2)}$ followed by the outgoing waves in all the channels. The functions $\psi^{(i)}$, $\chi_d^{(i)}$ and $\chi_p^{(i)}$ ($i=1$ and 2) are not well defined by Eqs. (2·13) through (2·14b). Only the asymptotic forms have been specified precisely because the variational expression will be obtained only through the asymptotic properties of these functions. A detailed discussion will be given in § 3 on some related ambiguities in defining the wave functions of relative motion. As will be shown there, the ambiguity can be avoided if we impose further appropriate conditions on these functions.

Let us now consider the following expression:

$$I_{12}(\boldsymbol{n}_1, -\boldsymbol{n}_2) = \int \Psi^{(2)*}(H-E)\Psi^{(1)}d\tau\,. \tag{2·15}$$

It should be remarked that $\Psi^{(2)*}$ is the time reversed wave function of $\Psi^{(2)}$. This point is important when the spins are considered in the variational formulation. If one gives infinitesimal variations to the wave functions $\Psi^{(1)}$ and $\Psi^{(2)}$ through variations in $\chi_d^{(i)}$, $\chi_p^{(i)}$ and $\psi^{(i)}$ $(i=1, 2)$, the variation of I_{12},

$$\delta I_{12} = \int \Psi^{(2)*}(H-E)\delta\Psi^{(1)}d\tau + \int \delta\Psi^{(2)*}(H-E)\Psi^{(1)}d\tau\,,$$

can be written as*)

$$\begin{aligned}\delta I_{12}(\boldsymbol{n}_1, -\boldsymbol{n}_2) &= \int \Psi^{(2)*}(H-E)\delta\Psi^{(1)}d\tau - \int \delta\Psi^{(1)}(H-E)\Psi^{(2)*}d\tau \\ &= -a_d\int \Psi^{(2)*}\Delta_R|_{np}\Phi^A\phi_d\delta\chi_d^{(1)}(\boldsymbol{R})\,d\tau_1 + a_d\int \Phi^A\phi_d\delta\chi_d^{(1)}(\boldsymbol{R})\,\Delta_R|_{np}\Psi^{(2)*}d\tau_1 \\ &\quad - a_p\int \Psi^{(2)*}\Delta_r|_n\Phi^B\delta\chi_p^{(1)}(\boldsymbol{r})\,d\tau_2 + a_p\int \Phi^B\delta\chi_p^{(1)}(\boldsymbol{r})\,\Delta_r|_n\Psi^{(2)*}d\tau_2 \\ &\quad + \int \Psi^{(2)*}(H-E)\delta\psi^{(1)}d\tau - \int \delta\psi^{(1)}(H-E)\Psi^{(2)*}d\tau\,,\end{aligned} \tag{2·16a}$$

where $d\tau_1 = d\xi d\boldsymbol{r}_{np}d\boldsymbol{R}$ and $d\tau_2 = d\xi d\boldsymbol{r}_n d\boldsymbol{r}$, and the equations $(H-E)\Psi^{(1)}=0$ and $(H-E)\Psi^{(2)*}=0$ are used. The terms containing $\Delta_{np}|_R$ and $\Delta_n|_r$ have been dropped because the bound state functions $\phi_d(r_{np})$ and $\phi_n(\boldsymbol{r}_n)$, respectively, ensure the hermiticity of these operators.

Let us consider the first two terms on the right-hand side of (2·16a). Using Green's theorem one can transform these two terms into a difference of two surface integrals at infinity. However, Eq. (2·14a) shows that the complex conjugate of the first term of $\Psi^{(2)}$ in (2·14) has an asymptotic form proportional to e^{ikR}/R as R goes to infinity which, according to (2·13a), is the same as the asymptotic form of $\delta\chi_d^{(1)}$. Hence, the difference of the surface integrals vanishes and we get no contribution from this term of $\Psi^{(2)}$. Furthermore, the second term of $\Psi^{(2)}$ on the right-hand side of (2·14) does not contribute to the surface integral, either, since the product $\Phi^{B*}\phi_d$ vanishes at infinity. Similarly, one can readily see that $\psi^{(2)}$ does not contribute to the surface integral.

For the third and fourth terms on the right-hand side of (2·16a), one can again transform them into a difference of two surface integrals at infinity. Of the three terms in the expression (2·14) for $\Psi^{(2)}$ the first term does not contribute to the integral since the product $\phi_d^*\Phi^B$ vanishes when r goes to infinity. Similarly, the third term $\psi^{(2)}$ of $\Psi^{(2)}$ gives no contribution. The second term of $\Psi^{(2)}$, however, does give finite contribution to the integral. Similarly the last two terms on the right-hand side of (2·16a) can be shown to contribute nothing.

One gets altogether

*) We assume that the potentials are static and non-exchange type with finite range.

$$\delta I_{12}(\boldsymbol{n}_1, -\boldsymbol{n}_2) = -a_p \int |\Phi^B|^2 d\hat{\xi} d\boldsymbol{r}_n \int \left\{ \exp(ik_p \boldsymbol{n}^{(2)} \boldsymbol{r}) \frac{\partial}{\partial n_r} \frac{\exp(ik_p r)}{r} \right.$$

$$\left. - \frac{\exp(ik_p r)}{r} \frac{\partial}{\partial n_r} \exp(ik_p \boldsymbol{n}^{(2)} \boldsymbol{r}) \right\} \delta g^{(1)}(\boldsymbol{n}^{(1)}, \boldsymbol{n}) dS_r = 4\pi a_p \delta g^{(1)}(\boldsymbol{n}^{(1)}, -\boldsymbol{n}^{(2)}), \tag{2·16b}$$

where S_r is a surface at infinity in the $\boldsymbol{r}$-space and n_r stands for the outward normal to S_r.

From (2·16b) one immediately sees that if one defines a quantity $g_{st}^{(1)}$ by

$$g_{st}^{(1)}(\boldsymbol{n}^{(1)}, -\boldsymbol{n}^{(2)}) = g^{(1)}(\boldsymbol{n}^{(1)}, -\boldsymbol{n}^{(2)}) - (4\pi a_p)^{-1} \int \Psi^{(2)*}(H-E)\Psi^{(1)} d\tau , \tag{2·17}$$

its variation vanishes:

$$\delta g_{st}^{(1)}(\boldsymbol{n}^{(1)}, -\boldsymbol{n}^{(2)}) = 0 . \tag{2·18}$$

Hence, $g_{st}^{(1)}$ is a stationary expression for $g^{(1)}$.

Conversely, the condition that $g_{st}^{(1)}$ is stationary at $\Psi^{(1)}$ and $\Psi^{(2)}$ leads to the Schrödinger equations for $\Psi^{(1)}$ and $\Psi^{(2)}$. In fact, if one gives arbitrary infinitesimal variations to these functions one gets

$$0 = \delta g_{st}^{(1)} = \delta g^{(1)} - (4\pi a_p)^{-1} \left\{ \int \delta\Psi^{(2)*}(H-E)\Psi^{(1)} d\tau + \int \Psi^{(2)*}(H-E)\delta\Psi^{(1)} d\tau \right\}$$

$$= -(4\pi a_p)^{-1} \left\{ \int \delta\Psi^{(2)*}(H-E)\Psi^{(1)} d\tau + \int \delta\Psi^{(1)}(H-E)\Psi^{(2)*} d\tau \right\} \tag{2·19}$$

by the same procedure as in the derivation of (2·16b). Hence,

$$(H-E)\Psi^{(1)} = 0 \qquad \text{and} \qquad (H-E)\Psi^{(2)*} = 0 ,$$

since $\delta\Psi^{(1)}$ and $\delta\Psi^{(2)}$ are independent variations. Hence, we have obtained a variational principle which is equivalent to the Schrödinger equation. The stationary value of the expression, $g_{st}^{(1)}$, is just the required scattering amplitude of (d, p) reaction.*)

*) The corresponding variation principles for $g^{(2)}$, $f^{(1)}$ and $f^{(2)}$ can be constructed similarly. The stationary expression for $g^{(2)}$ is given by

$$g_{st}^{(2)}(\boldsymbol{n}^{(2)}, -\boldsymbol{n}^{(1)}) = g^{(2)}(\boldsymbol{n}^{(2)}, -\boldsymbol{n}^{(1)}) - (4\pi a_d)^{-1} \int \Psi^{(1)}(H-E)\Psi^{(2)*} d\tau .$$

The stationary expression for $f^{(1)}$ is obtained if one consideres the wave functions of the form, $\Psi^{(3)} = \Phi^A \phi_d \chi_d^{(3)} + \Phi^B \chi_p^{(3)} + \psi^{(3)}$, with the asymptotic form, $\chi_d^{(3)}(\boldsymbol{R}) \sim \{\exp(ik_d \boldsymbol{n}^{(3)} \cdot \boldsymbol{R}) + f^{(3)}(\boldsymbol{n}^{(3)}, \boldsymbol{n}) R^{-1} \cdot \exp(ik_d R)\}^*$ and $\chi_p^{(3)}(\boldsymbol{r}) \sim \{g^{(2)}(\boldsymbol{n}^{(3)}, \boldsymbol{n}') r^{-1} \exp(ik_p r)\}^*$. The function $\psi^{(3)}$ vanishes asymptotically in the d- and p-channels and has only incoming waves in the asymptotic region of all the other open channels. The expression is

$$f_{st}^{(1)}(\boldsymbol{n}^{(1)}, -\boldsymbol{n}^{(3)}) = f^{(1)}(\boldsymbol{n}^{(1)}, -\boldsymbol{n}^{(3)}) - (4\pi a_d)^{-1} \int \Psi^{(3)*}(H-E)\Psi^{(1)} d\tau .$$

Conversely, the variational principle for these expressions leads to the Schrödinger equation for arbitrary variations, and leads to the same equations as (2·21) if we assume the truncated wave functions as defined in (2·20).

The variational principle obtained above can now be applied to determine the best set of wave functions of relative motion, $\chi_d^{(i)}$ and $\chi_p^{(i)}$. If one, namely, takes as the trial functions the wave functions of the form

$$\Psi_t^{(1)} = \Phi^A \phi_d \chi_{d,t}^{(1)} + \Phi^B \chi_{p,t}^{(1)} \tag{2·20a}$$

and

$$\Psi_t^{(2)} = \Phi^A \phi_d \chi_{d,t}^{(2)} + \Phi^B \chi_{p,t}^{(2)}, \tag{2·20b}$$

one gets from the condition that $g_{s,t}^{(1)}$ be stationary against $\Psi_t^{(1)}$ and $\Psi_t^{(2)}$ induced by the variations in $\chi_{d,t}^{(i)}$ and $\chi_{p,t}^{(i)}$ $(i=1, 2)$ the following set of equations:

$$\int \Phi^{A*} \phi_d^* (H-E) \Psi_t^{(1)} d\xi d\boldsymbol{r}_{np} = 0, \tag{2·21a}$$

$$\int \Phi^{B*} (H-E) \Psi_t^{(1)} d\xi d\boldsymbol{r}_n = 0, \tag{2·21b}$$

$$\int \Phi^A \phi_d (H-E) \Psi_t^{(2)*} d\xi d\boldsymbol{r}_{np} = 0 \tag{2·21c}$$

and

$$\int \Phi^B (H-E) \Psi_t^{(2)*} d\xi d\boldsymbol{r}_n = 0 \tag{2·21d}$$

which determine the unknown functions $\chi_{d,t}^{(i)}$ and $\chi_{p,t}^{(i)}$ $(i=1$ and $2)$. That is, if one inserts (2·20a) into (2·21a) and (2·21b) and uses (2·1), (2·2) and (2·6) through (2·11) one has a set of coupled integro-differential equations for χ's,

$$\begin{aligned}&(-a_d \Delta_R|_{np} + U_{dA} - E_d)\chi_d \\ &\quad = -\int \phi_d^* [(-a_p \Delta_r|_n + U_{pB} - E_p) + (V_{np} + V_{pA} - U_{pB})] \phi_n \chi_p d\boldsymbol{r}_{np}\end{aligned} \tag{2·22}$$

and

$$\begin{aligned}&(-a_p \Delta_r|_n + U_{pB} - E_p)\chi_p \\ &\quad = -\int \phi_n^* [(-a_p \Delta_r|_n + U_{pB} - E_p) + (V_{np} + V_{pA} - U_{pB})] \phi_d \chi_d d\boldsymbol{r}_n,\end{aligned} \tag{2·23}$$

respectively, where

$$U_{dA} = \int \Phi^{A*} \phi_d^* (V_{pA} + V_{nA}) \Phi^A \phi_d d\xi d\boldsymbol{r}_{np} \tag{2·24a}$$

and

$$U_{pB} = \int \Phi^{B*} (V_{pA} + V_{np}) \Phi^B d\xi d\boldsymbol{r}_n, \tag{2·24b}$$

and the superscript (1) and the subscript t are now dropped. It is easy to see that exactly the same set of equations as (2·22) and (2·23) can be derived for $\chi_d^{(2)}$ and $\chi_p^{(2)}$ from (2·21c) and (2·21d), which shows that the form of the equa-

tions for χ's is independent of the boundary condition imposed on them.

The integral terms of Eqs. (2·22) and (2·23) represent the coupling of the initial and final channels and give rise to the (d, p)- and (p, d)-reaction amplitudes. In the post form of Born approximation, including DWBA, the interaction responsible for the reaction is $V_{np}+V_{pA}-U_{pB}$. This corresponds to discarding all but $V_{np}+V_{pA}-U_{pB}$ from the square brackets of the coupling integrals. The DWBA amplitude is obtained if one solves such a truncated equations by perturbation theory in the first order.

In the present treatment, however, this is no longer the case since we do not assume the validity of the first order perturbation calculation. We must also consider the other terms $-a_p(\Delta_r|_n+k_p^2)+U_{pB}(r_p)$, in the coupling integrals. This complication arises from the fact that the internal wave functions of the initial and final channels are not orthogonal to each other. Discussion of the effect of this non-orthogonality will be given in more detail in § 4.

Now, let us estimate the error in the scattering amplitude obtained from Eqs. (2·21). For this purpose it is convenient to use the method of finite variation. Let us designate in general the approximation for $\Psi^{(i)}$ by $\Psi_t^{(i)}$ and its error by $\Delta\Psi^{(i)}$:

$$\Delta\Psi^{(i)}=\Psi_t^{(i)}-\Psi^{(i)}. \tag{2·25}$$

Corresponding to (2·15), let us consider the quantity, $I_{12t}\equiv\int\Psi_t^{(2)*}(H-E)\Psi_t^{(1)}d\tau$. A little calculation similar to that which was used to derive Eq. (2·16a) shows that

$$\begin{aligned}I_{12t}&=\int\Psi^{(2)*}(H-E)\Psi_t^{(1)}d\tau+\int\Delta\Psi^{(2)*}(H-E)\Delta\Psi^{(1)}d\tau\\&=4\pi a_p\{g_t^{(1)}(\boldsymbol{n}^{(1)},-\boldsymbol{n}^{(2)})-g^{(1)}(\boldsymbol{n}^{(1)},-\boldsymbol{n}^{(2)})\}+\int\Delta\Psi^{(2)*}(H-E)\Delta\Psi^{(1)}d\tau\,,\end{aligned} \tag{2·26}$$

where $g_t^{(1)}$ is the reaction amplitude corresponding to the wave function $\Psi_t^{(1)}$. This is an exact expression. It is clear from (2·26) that $g_t^{(1)}-(4\pi a_p)^{-1}I_{12t}$ is a stationary expression for $g^{(1)}$ as defined in Eq. (2·17). Since $I_{12t}=0$ for $\Psi_t^{(1)}$ satisfying Eqs. (2·21), the calculated $g_t^{(1)}$ is given by

$$g_t^{(1)}(\boldsymbol{n}^{(1)},-\boldsymbol{n}^{(2)})=g^{(1)}(\boldsymbol{n}^{(1)},-\boldsymbol{n}^{(2)})-(4\pi a_p)^{-1}\int\Delta\Psi^{(2)*}(H-E)\Delta\Psi^{(1)}d\tau \tag{2·27}$$

which shows that the error in the calculated amplitude $g_t^{(1)}$ is of the second order in $\Delta\Psi^{(i)}$. Expressions similar to (2·27) can be easily obtained for the other reaction- and elastic scattering amplitudes.

2.2 *Partial wave expansion*

Let us now consider general cases with $l_n\neq0$ in terms of the partial wave

expansion. We neglect the intrinsic spins of nucleons so that the total orbital angular momentum, which we designate by L, is a good quantum number. The total wave function Ψ_{LM} with the total orbital angular momentum L and its z component M can be written as

$$\Psi_{LM}=\Phi^{A}_{00}(\xi)\,\phi_d(r_{np})\,Y_{LM}(\hat{\boldsymbol{R}})\frac{u_L(R)}{R}$$
$$+\sum_{l=|L-l_n|}^{L+l_n}[\Phi^{B}_{l_n}(\xi,\boldsymbol{r}_n),\,Y_l(\hat{\boldsymbol{r}})]_{LM}\frac{v_l^{(L)}(r)}{r}+\psi_{LM}\,, \tag{2·28}$$

where

$$[\Phi_{l_n},\,Y_l]_{LM}=\sum_{m_n m}(l_n l m_n m|LM)\,\Phi_{l_n m_n}Y_{lm}\,, \tag{2·29}$$

and ψ_{LM} vanishes asymptotically in the d- and p-channels and has only outgoing waves in the asymptotic region of all the other open channels.*) It is clear from the rotational invariance of the Hamiltonian that u_L and $v_l^{(L)}$ are independent of M.

Let us first seek for a variational expression which will give the reaction amplitude, $T^{(L)}_{pl,dL}$, corresponding to the incident wave in the deuteron channel with the angular momentum L and the outgoing wave in the proton channel with the angular momentum l. For this purpose, let us consider a wave function $\Psi^{(1)}_{LM}$, which has the asymptotic form of an incident wave in the deuteron channel L plus outgoing waves in all the channels. We also consider a wave function $\Psi^{(2)}_{LM}$ which has the asymptotic form of an incident wave in the proton channel l plus incoming waves in all the channels. The corresponding radial wave functions, then, have the asymptotic forms,

$$\begin{aligned}&u_L^{(1)}(R)\sim\zeta_L^{\,d}F_L(k_d,\,R)+\zeta_L^{\,d}T^{(L)}_{dL,dL}\,H_L^{(+)}(k_d,\,R)\,,\\&v_{l'}^{(1)}(r)\sim\zeta^p_{l'}T^{(L)}_{pl',dL}H_{l'}^{(+)}(k_p,\,r)\end{aligned} \tag{2·30}$$

and

$$\begin{aligned}&u_L^{(2)}(R)\sim\{\zeta_L^{\,d}T^{(L)}_{dL,pl}H_L^{(+)}(k_d,\,R)\}^*\,,\\&v_{l''}^{(2)}(r)\sim\{\zeta^p_{l''}F_{l''}(k_p,\,r)\delta_{ll''}+\zeta^p_{l''}T^{(L)}_{pl'',pl}H_{l''}^{(+)}(k_p,\,r)\}^*\,,\end{aligned} \tag{2·31}$$

respectively, the superscript (L) on $v_l^{(i)}$ is dropped. Here F_L and $H_L^{(\pm)}$ are the regular and outgoing (incoming) wave Coulomb functions[35] whose asymptotic forms are given by

$$F_L(k,\,r)\sim\sin[kr-\eta\ln(2kr)-L\pi/2+\sigma_L]$$

and (2·32)

$$H_L^{(\pm)}(k,\,r)\sim\exp\{\pm i[kr-\eta\ln(2kr)-L\pi/2+\sigma_L]\}\,,$$

*) The comment on the ambiguity in defining ψ, χ_d and χ_p in (2·13) and (2·14) is applicable here. See also §3.

respectively, where

$$\zeta_L^{\,d}=i^L\exp(i\sigma_L^{\,d})/\sqrt{v_d} \qquad \text{and} \qquad \zeta_l^{\,p}=i^l\exp(i\sigma_l^{\,p})/\sqrt{v_p}\,, \tag{2·33}$$

with $v_d=\hbar k_d/\mu_d$ and $v_p=\hbar k_p/\mu_p$, and $\sigma_L^{\,d}=\arg\Gamma(1+L+i\eta_d)$ and $\sigma_l^{\,p}=\arg\Gamma(1+l+i\eta_p)$ are Coulomb phase shifts where $\eta_d=Ze^2\mu_d/\hbar^2k_d$ and $\eta_p=Ze^2\mu_p/\hbar^2k_p$, Ze being the charge of the target nucleus.

Let us designate approximate wave functions corresponding to $\Psi_{LM}^{(i)}$ by $\Psi_t^{(i)}$ and the corresponding error by

$$\Delta\Psi^{(i)}=\Psi_t^{(i)}-\Psi_{LM}^{(i)}\,. \tag{2·34}$$

In order to derive a stationary expression for the scattering amplitude, let us now calculate the integral $\int\Psi_t^{(2)*}(H-E)\Psi_t^{(1)}d\tau$. By a procedure similar to that used in deriving Eq. (2·26), one gets (see the Appendix)

$$\int\Psi_t^{(2)*}(H-E)\Psi_t^{(1)}d\tau=\int\Psi_{LM}^{*(2)}(H-E)\Psi_t^{(1)}d\tau+\int\Delta\Psi^{(2)*}(H-E)\Delta\Psi^{(1)}d\tau$$

$$=k_pa_p(\zeta_l^{\,p})^2T_{pl,dL,t}^{(L)}-k_da_d(\zeta_L^{\,d})^2T_{dL,pl}^{(L)}+\int\Delta\Psi^{(2)*}(H-E)\Delta\Psi^{(1)}d\tau\,. \tag{2·35}$$

If one substitutes $\Psi^{(1)}$ for $\Psi_t^{(1)}$ in (2·35) one gets, with the aid of (2·33)

$$(-1)^l\exp(2i\sigma_l^{\,p})\,T_{pl,dL}^{(L)}=(-1)^L\exp(2i\sigma_d^{\,L})\,T_{dL,pl}^{(L)}\,. \tag{2·36}$$

Since the S-matrix elements for (d,p) and (p,d) reactions are given by

$$S_{pl,dL}^{(L)}=2i\exp(2i\sigma_l^{\,p})\,T_{pl,dL}^{(L)} \qquad \text{and} \qquad S_{dL,pl}^{(L)}=2i\exp(2i\sigma_L^{\,d})\,T_{dL,pl}^{(L)}\,, \tag{2·37}$$

respectively, one has

$$(-1)^lS_{pl,dL}^{(L)}=(-1)^LS_{dL,pl}^{(L)}\,, \tag{2·38}$$

which shows the symmetry of the S-matrix.

In terms of Eqs. (2·36) and (2·37), Eq. (2·35) can be rewritten as

$$S_{pl,dL,t}^{(L)}=S_{pl,dL}^{(L)}+(-1)^l4i\hbar^{-1}\left\{\int\Psi_t^{(2)*}(H-E)\Psi_t^{(1)}d\tau\right.$$

$$\left.-\int\Delta\Psi^{(2)*}(H-E)\Delta\Psi^{(1)}d\tau\right\}. \tag{2·39}$$

Equation (2·39) shows that if one defines a quantity $S_{pl,dL,st}^{(L)}$ by

$$S_{pl,dL,st}^{(L)}\equiv S_{pl,dL,t}^{(L)}-(-1)^l4i\hbar^{-1}\int\Psi_t^{(2)*}(H-E)\Psi_t^{(1)}d\tau\,, \tag{2·40}$$

the difference between this quantity and the correct $S_{pl,dL}^{(L)}$ is equal to $-(-1)^l4i\hbar^{-1}\int\Delta\Psi^{(2)*}(H-E)\Delta\Psi^{(1)}d\tau$ and, therefore, is of the second order in $\Delta\Psi$'s. Hence, $S_{pl,dL,st}^{(L)}$ is stationary against variations in Ψ_t's around the correct solutions of the Schrödinger equation. Converse of this statement is also true since if one gives infinitesimal variations to $\Psi_t^{(1)}$ and $\Psi_t^{(2)}$ the variation in $S_{pl,dL,st}^{(L)}$ is given by

$$\delta S^{(L)}_{pl,dL,st}=$$

$$\delta S^{(L)}_{pl,dL,t}-(-1)^l 4i\hbar^{-1}\left\{\int \delta\Psi_t^{(2)*}(H-E)\Psi_t^{(1)}d\tau+\int \Psi_t^{(2)*}(H-E)\delta\Psi_t^{(1)}d\tau\right\}$$

$$=(-1)^{l+1}4i\hbar^{-1}\left\{\int \delta\Psi_t^{(2)*}(H-E)\Psi_t^{(1)}d\tau+\int \delta\Psi_t^{(1)}(H-E)\Psi_t^{(2)*}d\tau\right\}, \quad (2\cdot41)$$

and so the condition that $\delta S^{(L)}_{pl,dL,st}=0$ leads to the Schrödinger equations,

$$(H-E)\Psi_t^{(1)}=0\,, \qquad (H-E)\Psi_t^{(2)*}=0\,. \quad (2\cdot42)$$

In order to derive approximate equations for $u_L^{(i)}$ and $v_l^{(i)}$ from the variational principle, let us now take as the trial wave function the sum of the wave functions in the deuteron and proton channels,

$$\Psi_t^{(i)}=\Phi_{00}^A(\hat{\xi})\,\phi_d(r_{np})\,Y_{L0}(\hat{\boldsymbol{R}})\,\frac{u_L^{(i)}(R)}{R}$$

$$+\sum_{l=|L-l_n|}^{L+l_n}[\Phi_{l_n}^B(\hat{\xi},\boldsymbol{r}_n),\,Y_l(\hat{\boldsymbol{r}})]_{L0}\frac{v_l^{(i)}(r)}{r}\,. \quad (2\cdot43)$$

The condition that $\delta S^{(L)}_{pL,dL,st}$ given by (2·41) is zero for arbitrary variations in $u_L^{(i)}$ and $v_l^{(i)}$ is equivalent to the equations

$$\int \Phi_{00}^{A*}\phi_d{}^*Y_{L0}^*(\hat{\boldsymbol{R}})\,(H-E)\Psi_t^{(i)}d\xi d\boldsymbol{r}_{np}d\hat{\boldsymbol{R}}=0\,, \quad (2\cdot44)$$

and

$$\int[\Phi_{l_n}^{B*}(\hat{\xi},\boldsymbol{r}_n),\,Y_l{}^*(\hat{\boldsymbol{r}})]_{L0}(H-E)\Psi_t^{(i)}d\xi d\boldsymbol{r}_n d\hat{\boldsymbol{r}}=0\,. \quad (2\cdot45)$$

It can immediately be seen that these equations are independent of (i) which specifies the boundary condition of the solution.

The solutions of Eqs. (2·44) and (2·45) satisfy

$$\int \Psi_t^{(2)*}(H-E)\Psi_t^{(1)}d\tau=0\,. \quad (2\cdot46)$$

Hence, Eq. (2·39) gives

$$S^{(L)}_{pl,dL,t}=S^{(L)}_{pl,dL}+(-1)^{l+1}4i\hbar^{-1}\int \Delta\Psi^{(2)*}(H-E)\Delta\Psi^{(1)}d\tau\,, \quad (2\cdot47)$$

which shows that the error contained in the calculated S-matrix elements is of the order of the product of $\Delta\Psi^{(1)}$ and $\Delta\Psi^{(2)}$.

Using Eqs. (2·1) and (2·2) one can rewrite Eq. (2·44) as

$$-\frac{a_d}{R}\left\{\frac{d^2}{dR^2}+k_d{}^2-\frac{L(L+1)}{R^2}\right\}u_L(R)+U_{dA}(R)\,\frac{u_L(R)}{R}$$

$$+\int \Phi_{00}^{A*}\phi_d{}^*Y_{L0}^*(\hat{\boldsymbol{R}})\,[\{-a_p(\Delta_r|_n+k_p{}^2)+U_{pB}\}+\{V_{pA}(r_p{}')$$

$$+V_{np}(r_{np})-U_{pB}\}]\sum_l[\Phi_{ln}^B(\xi,\boldsymbol{r}_n),\ Y_l(\hat{\boldsymbol{r}})]_{L0}\frac{v_l(r)}{r}d\xi d\boldsymbol{r}_{np}d\hat{\boldsymbol{R}}=0\,, \qquad (2\cdot48)$$

and Eq. (2·45) as

$$-\frac{a_p}{r}\left\{\frac{d^2}{dr^2}+k^2{}_p-\frac{l(l+1)}{r^2}\right\}v_l(r)+U_{pB}(r)\frac{v_l(r)}{r}$$
$$+\int[\Phi_{ln}^{B*}(\xi,\boldsymbol{r}_n),\ Y_l^*(\hat{\boldsymbol{r}})]_{L0}[\{-a_p(\Delta_r|_n+k_p{}^2)+U_{pB}\}+\{V_{pA}(r_p{}')$$
$$+V_{np}(r_{np})-U_{pB}\}]\Phi_{00}^A(\xi)\phi_d(r_{np})Y_{L0}(\hat{\boldsymbol{R}})\frac{u_L(R)}{R}d\xi d\boldsymbol{r}_n d\hat{\boldsymbol{r}}=0\,, \qquad (2\cdot49)$$

where the superscript (i) is dropped and

$$U_{dA}(R)=\int\Phi_{00}^{A*}(\xi)\phi_d{}^*(r_{np})Y_{L0}^*(\hat{\boldsymbol{R}})\{V_{nA}(r_n)$$
$$+V_{pA}(r_p{}')\}\Phi_{00}^A(\xi)\phi_d(r_{np})Y_{L0}(\hat{\boldsymbol{R}})d\xi d\boldsymbol{r}_{np}d\hat{\boldsymbol{R}} \qquad (2\cdot50)$$

and

$$U_{pB}(r)=\int[\Phi_{ln}^{B*}(\xi,\boldsymbol{r}_n),\ Y_l^*(\hat{\boldsymbol{r}})]_{L0}\{V_{pA}(r_p{}')$$
$$+V_{np}(r_{np})\}[\Phi_{ln}^B(\xi,\boldsymbol{r}_n),\ Y_l(\hat{\boldsymbol{r}})]_{L0}d\boldsymbol{r}_n d\hat{\boldsymbol{r}}d\xi\,, \qquad (2\cdot51)$$

which are distorting potentials in the deuteron and proton channels respectively. Equations (2·48) through (2·51) constitute the basic equations of the present method. These equations contain the derivatives of the unkown functions $u_L(R)$ and $v_l(r)$ in the interaction kernel, which is very inconvenient for the practical calculation. Fortunately, however, as will be shown in a subsequent paper, these derivatives can be eliminated from the integral kernels, putting at the same time the two kernels in exactly the same form. The S-matrix elements are then also shown to be symmetrical with respect to the initial and final channels.

Strictly speaking, Eqs. (2·49) and (2·51) are correct only when the captured neutron goes into an s-orbit. In fact, from (2·2) and (2·28) one immediately sees that the part of the integral in (2·45) which is relevant to U_{pB} is

$$\int[\Phi_{ln}^{B*}(\xi,\boldsymbol{r}_n),\ Y_l^*(\hat{\boldsymbol{r}})]_{L0}\left[V_{pA}\left(\left|\frac{\boldsymbol{r}_n}{A+1}+\boldsymbol{r}\right|\right)+V_{np}\left(\left|\frac{A}{A+1}\boldsymbol{r}_n-\boldsymbol{r}\right|\right)\right]$$
$$\times\sum_{l'}[\Phi_{ln}^B(\xi,\boldsymbol{r}_n),\ Y_{l'}(\hat{\boldsymbol{r}})]_{L0}d\xi d\boldsymbol{r}_n d\hat{\boldsymbol{r}}\frac{v_{l'}(r)}{r}\,. \qquad (2\cdot52)$$

If the integrals over ξ and $\boldsymbol{r}_n$ result in an integrand which is a function only of r, the integral over $\hat{\boldsymbol{r}}$ vanishes unless $l=l'$ and the above integral reduces to

$$\int[\Phi_{ln}^{B*},\ Y_l^*]_{L0}(V_{pA}+V_{np})[\Phi_{ln}^B,\ Y_l]_{L0}d\xi d\boldsymbol{r}_n d\hat{\boldsymbol{r}}\frac{v_l(r)}{r}$$

from which (2·49) and (2·51) follow. If l_n is different from zero, however, the above argument no longer holds and one may have to deal with much more complicated equations than (2·49) and (2·51). None the less, these are presumably good approximations if the target nucleus A is sufficiently large, and we shall henceforth assume that (2·49) and (2·51) are valid.

So far, we have entirely neglected the effect of the channels other than the strongly coupled initial and final channels. One could take this effect into account by adding to the trial wave functions the sum of wave functions in those channels. Equations (2·48) and (2·49) would then get extra terms corresponding to the additional terms in the trial wave function, but we content ourselves here with the assumption that the effect of the additional terms may be taken into account at least partly by replacing U_{pB} and U_{dA} by some phenomenological complex potentials which we again denote by U_{pB} and U_{dA} respectively. The coupling kernels also will then be modified and have the imaginary part (see § 3). The best choice of the potentials, U_{pB} and U_{dA}, will be determined by adjusting the parameters to cope with experiment.

We have, up to now, considered the variational method for calculating the special S-matrix element, $S^{(L)}_{pl,dL}$. In the same way, one can set up a variational principle for a general S-matrix element, $S^{(L)}_{\beta\alpha}$, if one takes for $\Psi^{(1)}$ in the above discussions the total wave function whose asymptotic form is an incident wave in the channel α plus outgoing waves in all the channels and for $\Psi^{(2)}$ the wave function which has the asymptotic form of an incident wave in the channel β plus incoming waves in all the channels. One then gets the basic equations which are exactly the same as (2·48) and (2·49). For the S-matrix element $S^{(L)}_{\beta\alpha,t}$, which is obtained from the solutions of these equations, one gets an equation of the same form as (2·47),

$$S^{(L)}_{\beta\alpha,t}=S^{(L)}_{\beta\alpha}+(-1)^{l_\beta+1}4i\hbar^{-1}\int \Delta\Psi^{(2)*}(H-E)\,\Delta\Psi^{(1)}d\tau\,. \tag{2·53}$$

Thus, we see that the solutions to Eqs. (2·48) and (2·49) give rise to a stationary value of the S-matrix element.

2.3 *Cross section*

Solving the coupled equations (2·48) and (2·49), one gets the wave function of the form (2·28) and the reaction amplitude, $T^{(L)}_{\beta\alpha}$, defined by (2·30) and (2·31) from which the S-matrix element is given by

$$S^{(L)}_{\beta\alpha}=\exp(2i\sigma_\beta)\,(\delta_{\beta\alpha}+2iT^{(L)}_{\beta\alpha})\,. \tag{2·54}$$

The practical method of computing the S-matrix elements will be described in the subsequent paper.

The differential cross sections are given for the (d, p) reaction by

$$\sigma_{dp}=\frac{\pi}{k_d^{\,2}}\sum_m\Big|\sum_{Ll}\sqrt{2L+1}\,(l_n lm-m|L0)\,S^{(L)}_{pl,dL}Y_{l-m}(\theta,\phi)\Big|^2 \tag{2·55}$$

and for the (p, d) reaction by

$$\sigma_{pd}=\frac{\pi}{(2l_n+1)k_p{}^2}\sum_m|\sum_{lL}\sqrt{2l+1}\,(l_nlm0|Lm)S^{(L)}_{dL,pl}Y_{Lm}(\theta,\phi)|^2. \qquad (2\cdot56)$$

The condition of detailed balance is

$$(2l_n+1)k_p{}^2\sigma_{pd}=k_d{}^2\sigma_{dp}\,.$$

The elastic scattering cross sections are given for the (d, d) process by

$$\sigma_{dd}=|f_d(\theta)+\frac{\sqrt{4\pi}}{k_d}\sum_L\sqrt{2L+1}\exp(2i\sigma_L{}^d)T^{(L)}_{dL,dL}Y_{L0}(\theta,\phi)|^2 \qquad (2\cdot57)$$

and for (p, p) by

$$\sigma_{pp}=\frac{1}{(2l_n+1)}\sum_{mm'}|f_p(\theta)\delta_{m'0}+\frac{\sqrt{4\pi}}{k_p}\sum_{Lll'}\sqrt{2l+1}\exp(2i\sigma^p_{l'})$$
$$\times(l_nl'm-m'm'|Lm)(l_nlm0|Lm)T^{(L)}_{pl',pl}Y_{l'm'}(\theta,\phi)|^2, \qquad (2\cdot58)$$

where $f_d(\theta)$ and $f_p(\theta)$ are the Rutherford scattering amplitude in the deuteron and proton channels, respectively.

§ 3. Ambiguities in the wave functions and effective Hamiltonian, and the relation to projection operator methods

We have pointed out in § 2.1 that Eqs. (2·13) and the boundary conditions are not enough to define χ_d, χ_p and ψ. Let the wave function Ψ be written in the form

$$\Psi=\sum_{\alpha=1}^{N}\Phi_\alpha\chi_\alpha+\psi\,, \qquad (3\cdot1)$$

where Φ_α is the internal wave function of the channel α which consists of a pair of particles and χ_α is the corresponding wave function of relative motion. Then, the boundary condition in the asymptotic region is not enough to determine the χ's and ψ uniquely. For, any simultaneous replacement of χ_α by $\chi_\alpha+\Delta\chi_\alpha$ and ψ by $\psi-\Phi_\alpha\Delta\chi_\alpha$ with arbitrary function $\Delta\chi_\alpha$ which vanishes in the asymptotic region would give a different but equally valid expression for Ψ of the form of (3·1). The ambiguity may be eliminated only when further suitable conditions are imposed on the χ's and ψ.

For inelastic scattering, the "most natural" condition is that ψ be orthogonal to each term in the sum on the right-hand side of (3·1). In fact, if one supposes that Ψ is expanded in the complete set of internal wave functions of the colliding pair, Eq. (3·1) would be obtained by picking out the terms corresponding to some closely coupled channels in the form of a sum and putting the rest equal to ψ. Since the internal wave function contained in ψ are orthogonal to those in the sum, the above condition is fulfilled. Conversely, this condition

determines the χ's and ψ uniquely.

For a rearrangement reaction, however, there is no such unique "natural" condition. There is even no unique expansion of Ψ in a complete set such as considered above for inelastic scattering. In fact, for the (d, p) reaction, for instance, there are two complete sets of internal states corresponding respectively to the initial $d+A$ and final $p+B$ systems. The total wave function Ψ could be expanded in either of the two sets or any linear combination thereof. Expansion of Ψ in both of these sets, which might be suggested by the form of (2·13), would not be unique since the basis is overcomplete.

Thus, for the case in § 2 one could still assume as a "natural" condition that ψ be orthogonal to the first two terms on the right-hand side of Eq. (2·13) or (2·14) for arbitrary χ_d and χ_p,

$$\int \Phi^{A*}\phi_d{}^*\psi d\xi d\boldsymbol{r}_{np}=0\,, \qquad \int \Phi^{B*}\psi d\xi d\boldsymbol{r}_n=0\,. \tag{3·2}$$

This condition is consistent with the required asymptotic form of ψ and defines χ_d, χ_p and ψ uniquely, as will be seen in the following. Alternatively, one could impose another, equally "natural" condition that the χ's and ψ be defined by the projection operators,

$$P_d=|\Phi^A\phi_d\rangle\langle\Phi^A\phi_d| \qquad \text{and} \qquad P_p=|\Phi^B\rangle\langle\Phi^B|\,, \tag{3·3}$$

through

$$\Phi^A\phi_d\chi_d=P_d\Psi\,, \qquad \Phi^B\chi_p=P_p\Psi \tag{3·4}$$

and

$$\psi=(1-P_d-P_p)\Psi\,. \tag{3·5}$$

We can readily observe that the latter definition is different from the former one, (3·2): $P_d\psi=0$ and $P_p\psi=0$, since we have

$$P_d\psi=-P_dP_p\Psi \qquad \text{and} \qquad P_p\psi=-P_pP_d\Psi\,, \tag{3·6}$$

which are in general different from zero because of the "*non-orthogonality*" of p and d channels. We also see that χ_d, χ_p and ψ defined by (3·3) through (3·5) have correct asymptotic behaviour since

$$\lim_{R\to\infty}P_d\psi=-\lim_{R\to\infty}\Phi^A\phi_d\int d\xi d\boldsymbol{r}_{np}\Phi^{A*}(\xi)\phi_d{}^*(\boldsymbol{r}_{np})\Phi^B(\xi,\boldsymbol{r}_n)\int d\xi' d\boldsymbol{r}_n{}'\Phi^{B*}(\xi',\boldsymbol{r}_n{}')\Psi=0$$

and

$$\lim_{r\to\infty}P_p\psi=-\lim_{r\to\infty}\Phi^B\int d\xi d\boldsymbol{r}_n\Phi^{B*}(\xi,\boldsymbol{r}_n)\Phi^A(\xi)\phi_d(\boldsymbol{r}_{np})\int d\xi' d\boldsymbol{r}'_{np}\Phi^{A*}(\xi')\phi_d{}^*(\boldsymbol{r}'_{np})\Psi=0\,.$$

There may be still other "natural" conditions to define χ_d, χ_p and ψ depending on the aim of the formulation.

It is clear that Eq. (3·4) uniquely defines χ_d and χ_p, but is not so clear

with the orthogonality conditions (3·2). Let us, therefore, examine if these are sufficient to eliminate the ambiguity. If there are still ambiguities $\Delta\chi_d$, $\Delta\chi_p$ and $\Delta\psi$ in χ_d, χ_p and ψ respectively, they must satisfy

$$\Phi^A\phi_d\Delta\chi_d+\Phi^B\Delta\chi_p+\Delta\psi=0\,. \tag{3·7}$$

Using the condition that $\Delta\psi$ be orthogonal to the first two terms on the left-hand side of (3·7) one gets

$$\Delta\chi_p(\boldsymbol{r})+\int K_1(\boldsymbol{r},\boldsymbol{R})\Delta\chi_d(\boldsymbol{R})\,d\boldsymbol{R}=0 \tag{3·8}$$

and

$$\Delta\chi_d(\boldsymbol{R})+\int K_2(\boldsymbol{R},\boldsymbol{r})\Delta\chi_p(\boldsymbol{r})\,d\boldsymbol{r}=0\,, \tag{3·9}$$

where

$$K_1(\boldsymbol{r},\boldsymbol{R})=K_2^*(\boldsymbol{R},\boldsymbol{r})=8\phi_n^*(2\boldsymbol{R}-\boldsymbol{r})\phi_d(2\boldsymbol{R}-2\boldsymbol{r}) \tag{3·10}$$

and

$$\phi_n=\int\Phi^{A*}\Phi^B d\hat{\xi}\,,$$

for infinitely heavy target nucleus. Equations (3·8) through (3·10) are a special case of Mittleman's eigenvalue equation with the eigenvalue $\lambda=1$ (see (3·17)). Conversely, if these equations have non-trivial solutions, there exist non-zero $\Delta\chi_d$ and $\Delta\chi_p$ such that $\Phi^A\phi_d\Delta\chi_d+\Phi^B\Delta\chi_p=0$ so that the conditions (3·2) are not adequate to remove the ambiguity.[21] Whether or not this actually happens depends on the structure of Φ^A and Φ^B, but as Coz' has shown,[21] it happens in such a very special case*) that one could safely ignore the possibility in most practical cases.

The ambiguity which has been discussed so far does not necessarily give rise to the ambiguity in $\chi_{d,t}(u_L^{(i)})$ and $\chi_{p,t}(v_l^{(i)})$ in the trial function in Eq. (2·20) (Eq. (2·43)) adopted in the present paper. As long as the solution for Ψ_t of the variational procedure is unique, the ambiguity in $\chi_{d,t}$ and $\chi_{p,t}$ will remain only in the very special case when exactly the same equations as Eqs. (3·8) through (3·10) are satisfied.

The same thing will be true more generally if the trial wave function is a sum of wave functions of any finite number of strongly coupled channels.

Let us now turn to the discussion of the effective Hamiltonian introduced in § 2.2. We have assumed there that the effect of the eliminated channels are taken into account by making the potentials U_{dA} and U_{pB} complex and adjustable so that the experiments are best reproduced by the theory. This point can be further elucidated with the aid of the projection operator techniques[20)~22),26] de-

*) All the possible forms of Eqs. (3·8) through (3·10) with non-trivial solutions have been explicitly given in the Appendix of reference 21).

veloped in recent years. Therefore, let us first discuss the relation between the present method and the method of projection operators.

Let us first consider the formalism given by Mittleman.[20] A projection operator Π is defined by

$$\int d\xi d\boldsymbol{r}_n \Phi^{B*}\Phi = \int d\xi d\boldsymbol{r}_n \Phi^{B*}\Pi\Phi\,, \tag{3·11}$$

and

$$\int d\xi d\boldsymbol{r}_{np} \Phi^{A*}\phi_d{}^*\Phi = \int d\xi d\boldsymbol{r}_{np} \Phi^{A*}\phi_d{}^*\Pi\Phi\,, \tag{3·12}$$

for any Φ. If χ_d and χ_p are defined by

$$\Pi\Psi = \Phi^A\phi_d\chi_d + \Phi^B\chi_p\,,$$

the conditions (3·2) immediately follow. With the use of the projection operator $Q=1-\Pi$ the Schrödinger equation

$$[E-H]\Psi = 0 \tag{3·13}$$

can be put in a form

$$[E-H_{\rm eq}]\Pi\Psi = 0\,, \qquad H_{\rm eq} = \Pi H'\Pi\,, \tag{3·14}$$

where

$$H' = H + HQ(E-QHQ)^{-1}QH\,. \tag{3·15}$$

The explicit form of the projection operator Π is given by

$$\begin{aligned}\Pi(\boldsymbol{r}, \boldsymbol{r}_n; \boldsymbol{r}', \boldsymbol{r}_n') &= \phi_n(\boldsymbol{r}_n)\left[\delta(\boldsymbol{r}-\boldsymbol{r}') + \sum_{\lambda\neq 1}\frac{v_\lambda(\boldsymbol{r})v_\lambda{}^*(\boldsymbol{r}')}{\lambda^2-1}\right]\phi_n{}^*(\boldsymbol{r}_n') \\ &+ \phi_d(\boldsymbol{r}_{np})\left[\delta(\boldsymbol{R}-\boldsymbol{R}') + \sum_{\lambda\neq 1}\frac{u_\lambda(\boldsymbol{R})u_\lambda{}^*(\boldsymbol{R}')}{\lambda^2-1}\right]\phi_d{}^*(\boldsymbol{r}_{np}') \\ &- \phi_n(\boldsymbol{r}_n)K_1(\boldsymbol{r}, \boldsymbol{R}')\phi_d{}^*(\boldsymbol{r}_{np}') - \phi_d(\boldsymbol{r}_{np})K_2(\boldsymbol{R}, \boldsymbol{r}')\phi_n{}^*(\boldsymbol{r}_n') \\ &+ \sum_{\lambda\neq 1}\lambda^{-1}(\lambda^2-1)^{-1}[\phi_n(\boldsymbol{r}_n)v_\lambda(\boldsymbol{r})u_\lambda{}^*(\boldsymbol{R}')\phi_d{}^*(\boldsymbol{r}_{np}') + \phi_d(\boldsymbol{r}_{np})u_\lambda(\boldsymbol{R})v_\lambda{}^*(\boldsymbol{r}')\phi_n{}^*(\boldsymbol{r}_n')],\end{aligned} \tag{3·16}$$

where v_λ and u_λ are the solutions of the following eigenvalue equations,

$$\begin{aligned} v_\lambda(\boldsymbol{r}) + \lambda\int K_1(\boldsymbol{r}, \boldsymbol{R})u_\lambda(\boldsymbol{R})d\boldsymbol{R} = 0\,, \\ u_\lambda(\boldsymbol{R}) + \lambda\int K_2(\boldsymbol{R}, \boldsymbol{r})v_\lambda(\boldsymbol{r})d\boldsymbol{r} = 0\,. \end{aligned} \tag{3·17}$$

The effective Hamiltonian $H_{\rm eq}$ is a complicated, non-local operator as Eqs. (3·14), (3·15) and (3·16) show. This is so even if Q is put equal to zero as is done in a truncated theory, and at first sight Eq. (3·14) looks hardly related to our basic equations, (2·22) and (2·23). However, the non-locality in the truncated theory is only apparent as we shall show. One gets from Eq. (3·14)

$$\int d\xi d\boldsymbol{r}_n \Phi^{B*} \Pi [E-H'] \Pi \Psi = 0 , \tag{3·18}$$

where $\Pi^2=\Pi$ was used. If one takes $\Phi=H'\Pi\Psi$ in Eq. (3·11) of the definition of Π, one has

$$\int d\xi d\boldsymbol{r}_n \Phi^{B*} \Pi H' \Pi \Psi = \int d\xi d\boldsymbol{r}_n \Phi^{B*} H' \Pi \Psi .$$

Thus, Eq. (3·18) can be rewritten as

$$\int d\xi d\boldsymbol{r}_n \Phi^{B*} [E-H'] \Pi \Psi = 0 . \tag{3·19}$$

Similarly, one can derive the equation

$$\int d\xi d\boldsymbol{r}_{np} \Phi^{A*} \phi_d^* [E-H'] \Pi \Psi = 0 . \tag{3·20}$$

If one truncates other channels by putting $Q=0$ one eventually obtains (2·22) and (2·23). We assume in the actual calculation that the term in H' depending on Q can approximately be taken into account by a complex effective Hamiltonian with adjustable parameters as mentioned in § 2.2.

Next, let us consider the equation for χ_d and χ_p defined by Eq. (3·4). The projection operators P_d and P_p do not commute with each other so that $(1-P_d-P_p)$ is not a projection operator. It is therefore, difficult to derive equations satisfied by $P_d\Psi$ and $P_p\Psi$, i.e. χ_d and χ_p, by a straightforward application of Feshbach's technique.[26]

Let us introduce the projection operators Q_d and Q_p by

$$Q_d=1-P_d , \qquad Q_p=1-P_p , \tag{3·21}$$

and write the Schrödinger equation in the form

$$(H-E)(P_d+Q_d)\Psi+(H-E)(P_p+Q_p)\Psi=0 . \tag{3·22}$$

Eliminating $Q_d\Psi$ and $Q_p\Psi$ from the equations obtained by multiplying P_d, Q_d, P_p and Q_p, respectively, from the left of Eq. (3·22), one formally gets

$$\left[\hat{\boldsymbol{H}}-\hat{\boldsymbol{E}}+\boldsymbol{V}\boldsymbol{Q}\frac{1}{\boldsymbol{Q}(\hat{\boldsymbol{E}}-\hat{\boldsymbol{H}})\boldsymbol{Q}}\boldsymbol{Q}\boldsymbol{V}\right]\boldsymbol{P}\boldsymbol{\Psi}=0 , \tag{3·23}$$

where

$$\boldsymbol{P}=\begin{pmatrix} P_d & 0 \\ 0 & P_p \end{pmatrix}, \quad \boldsymbol{Q}=\begin{pmatrix} Q_d & 0 \\ 0 & Q_p \end{pmatrix}, \quad \boldsymbol{\Psi}=\begin{pmatrix} \Psi \\ \Psi \end{pmatrix},$$

$$\hat{\boldsymbol{H}}-\hat{\boldsymbol{E}}=(H-E)\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \tag{3·24}$$

and

$$\boldsymbol{V}=(\hat{\boldsymbol{H}}-\hat{\boldsymbol{E}})-\boldsymbol{P}(\hat{\boldsymbol{H}}-\hat{\boldsymbol{E}})\boldsymbol{P},$$

Equation (3·23) has exactly the same form as the equation derived by Hahn[22] by the projection operator method. The definition of Ψ in Hahn's theory is, however, different from the present one in that the sum of the components, but not the components themselves, is the total wave function. Each component corresponds to a definite colliding pair and has a finite amplitude in the asymptotic region of only elastic and inelastic channels of that pair.

If Q is put equal to zero Eq. (3·23) is reduced to our coupled channel equations (2·22) and (2·23), but to put Q equal to zero does not correspond to any simple type of truncation in Mittleman's formalism.

From the above discussions we see that the effective Hamiltonian is closely related to the definition of the projection operators which define χ_d and χ_p. In other words, there is an inherent ambiguity in the definition of the effective Hamiltonian associated with the ambiguity in the definition of the wave function.

In actual calculations, however, a phenomenological Hamiltonian such as the one discussed in § 2.2 is used. It is, therefore, impossible to know exactly to which definition of χ_d and χ_p such Hamiltonian and the calculated wave functions correspond. Since the behaviour of χ_d and χ_p in the internal region depends on the definition as we have seen, it is in general dangerous to draw a definite physical picture for the internal region from the analysis of such phenomenological wave functions.

§ 4. Effect of non-orthogonality and relation to DWBA

Let us investigate the effect of the non-orthogonality term on the S-matrix elements. In particular, let us pay attention to the limit of weak coupling in which the interaction term in the coupling integral, $V_{np}+V_{pA}-U_{pB}$, becomes very small. At first sight this assumption might appear to be equivalent to the assumption of DWBA. Actually, however, the two assumptions would be equivalent if the non-orthogonality term tended to zero faster than the interaction term, as will be seen below. This question, therefore, is closely related to the question of whether or not the present method is equivalent to DWBA in the weak coupling limit.

In order to avoid unnecessary complications due to angular momenta, let us again take up the simple example considered in § 2.1 in which l_n is zero. We also assume that the target nucleus is sufficiently heavy so that we can neglect the recoil of the residual nucleus and put

$$\boldsymbol{R}=\frac{\boldsymbol{r}+\boldsymbol{r}_n}{2} \qquad \text{and} \qquad \boldsymbol{r}_{np}=\boldsymbol{r}_n-\boldsymbol{r}\,. \tag{4·1}$$

The basic equations (2·22) and (2·23) are of the form

$$(K_d+U_{dA}-E_d)\chi_d(\boldsymbol{R})=-\int d\boldsymbol{r}_{np}\phi_d^*(\boldsymbol{r}_{np})\,[N+V]\phi_n\left(\boldsymbol{R}+\frac{\boldsymbol{r}_{np}}{2}\right)\chi_p\left(\boldsymbol{R}-\frac{\boldsymbol{r}_{np}}{2}\right), \tag{4·2}$$

$$(K_p+U_{pB}-E_p)\chi_p(\boldsymbol{r})=-\int d\boldsymbol{r}_n\phi_n^*(\boldsymbol{r}_n)\,[N+V]\,\phi_d(\boldsymbol{r}_n-\boldsymbol{r})\,\chi_d\left(\frac{\boldsymbol{r}_n+\boldsymbol{r}}{2}\right), \quad (4\cdot3)$$

where

$$K_d=-a_d\Delta_R|_{np}, \qquad K_p=-a_p\Delta_r|_n,$$
$$N=K_p+U_{pB}-E_p \quad \text{and} \quad V=V_{np}+V_{pA}-U_{pB}\,. \quad (4\cdot4)$$

The terms in the coupling integrals containing N are the non-orthogonality terms. Since N does not depend on $\boldsymbol{r}_n$, the integral on the right-hand side of (4·3) containing N is essentially the overlap integral of wave functions in d and p channels which does not vanish. Unfortunately, such an interpretation is not applicable to (4·2) and we shall discuss about it later in this section. The terms with V are the interaction terms which alone remain in DWBA.

Now, let us turn Eqs. (4·2) and (4·3) into a set of coupled integral equations by means of Green's functions $(E_d-K_d-U_{dA}+i\varepsilon)^{-1}$ and $(E_p-K_p-U_{pB}+i\varepsilon)^{-1}$ under the boundary condition that the asymptotic form of the wave function is an incident wave in the deuteron channel plus outgoing scattered waves. The resulting integral equations are, then,

$$\chi_d(\boldsymbol{R})=\chi_d^{(0)}(\boldsymbol{R}) + \frac{1}{E_d-K_d-U_{dA}+i\varepsilon}\int d\boldsymbol{r}_{np}\phi_d^*(\boldsymbol{r}_{np})\,[N+V]\,\phi_n\left(\boldsymbol{R}+\frac{\boldsymbol{r}_{np}}{2}\right)\chi_p\left(\boldsymbol{R}-\frac{\boldsymbol{r}_{np}}{2}\right) \quad (4\cdot5)$$

and

$$\chi_p(\boldsymbol{r})=-\int d\boldsymbol{r}_n\phi_n^*(\boldsymbol{r}_n)\,\phi_d(\boldsymbol{r}_n-\boldsymbol{r})\,\chi_d\left(\frac{\boldsymbol{r}_n+\boldsymbol{r}}{2}\right) + \frac{1}{E_p-K_p-U_{pB}+i\varepsilon}\int d\boldsymbol{r}_n\phi_n^*(\boldsymbol{r}_n)\,V\phi_d(\boldsymbol{r}_n-\boldsymbol{r})\,\chi_d\left(\frac{\boldsymbol{r}_n+\boldsymbol{r}}{2}\right), \quad (4\cdot6)$$

where $\chi_d^{(0)}$ is the solution of the homogeneous equation associated with Eq. (4·2) representing the incident plane wave plus an outgoing scattered wave due to U_{dA} alone in the deuteron channel.

Now, the reaction amplitude of the (d, p) process is obtained by considering the asymptotic form of $\chi_p(\boldsymbol{r})$ in the region of $r\to\infty$. In this region of $\boldsymbol{r}$ the first term on the right-hand side of Eq. (4·6) is zero since either $\phi_d(\boldsymbol{r}_n-\boldsymbol{r})$ or, if otherwise, $\phi_n(\boldsymbol{r}_n)$ vanishes. The second term, on the other hand, is finite and gives the matrix element for the (d, p) reaction,

$$S_{pd}\propto\iint\chi_p^{(0)*}(\boldsymbol{r})\,\phi_n^*(\boldsymbol{r}_n)\,V\phi_d(\boldsymbol{r}_n-\boldsymbol{r})\,\chi_d\left(\frac{\boldsymbol{r}_n+\boldsymbol{r}}{2}\right)d\boldsymbol{r}_n d\boldsymbol{r}\,, \quad (4\cdot7)$$

where $\chi_p^{(0)}$ is the solution of the homogeneous equation associated with Eq. (4·3) representing a plane wave plus an incoming scattered wave due to U_{pB} in the proton channel.

From Eq. (4·7) it is clear that S_{pd} becomes zero if V is put equal to zero,

which shows that the non-orthogonality term alone cannot give a finite S-matrix element for the (d, p) reaction. The same thing is true also for the (d, p) reaction amplitude because of the symmetry of the S-matrix.

Similarly, it is easy to show that in the weak coupling limit the (p, p) scattering amplitude reduces to the optical model value.

At first sight, the above arguments might seem to show that the non-orthogonality term has no effect at all on (d, p), (p, d) or (p, p) scattering amplitudes in the weak coupling limit. The latter statement is obviously correct for the (p, p) amplitude. For (d, p) and (p, d) amplitudes, however, one must be more careful since these amplitudes depend on χ_d as Eq. (4·7) shows.

In fact, Eqs. (4·5) and (4·6) reduce to

$$\chi_d = \chi_d^{(0)} - \frac{1}{E_d - K_d - U_{dA} + i\varepsilon} \int d\boldsymbol{r}_{np} \phi_d^*(\boldsymbol{r}_{np}) N \phi_n\left(\boldsymbol{R} - \frac{\boldsymbol{r}_{np}}{2}\right) \times \int d\boldsymbol{r}_n' \phi_n^*(\boldsymbol{r}_n') \phi_d\left(\boldsymbol{r}_n' - \boldsymbol{R} + \frac{\boldsymbol{r}_{np}}{2}\right) \chi_d\left(\frac{\boldsymbol{r}_n' + \boldsymbol{R}}{2} - \frac{\boldsymbol{r}_{np}}{4}\right), \tag{4·8}$$

in the limit $V \to 0$, of which the second term on the right-hand side gives a finite contribution in the asymptotic region. Hence, the non-orthogonality term gives a non-vanishing contribution to the (d, d) scattering amplitude even in the limit $V \to 0$. It, then, follows from (4·8) that S_{pd} is also affected by the non-orthogonality term through χ_d. Hence, we see that the (d, d), (p, d) and (d, p) reaction amplitudes calculated by the present method do not agree with those of DWBA even in the weak coupling limit.

The reason for this discrepancy stems from the fact that the division of the interaction kernel into the non-orthogonality term and the interaction term is actually not unique. In fact, in the prior form of the Hamiltonian the non-orthogonality term and the interaction term would be, respectively,

$$N' = K_d + U_{dA} - E_d \quad \text{and} \quad V' = V_{nA} + V_{pA} - U_{dA}. \tag{4·9}$$

It is easy to show that the scattering amplitude of (d, d) reduces to the optical model value as V' tends to zero. However, V' does not vanish in the limit $V \to 0$, and so χ_d does not tend to the optical model wave function in this limit. Similarly, if one defines the weak coupling limit by $V' \to 0$ one would get the optical model wave function in this limit for χ_d but not for χ_p.

Thus, we conclude that the present method is not equivalent to DWBA because of the non-orthogonality term even in the weak coupling limit in the sense that either V or V' is very weak. In the solution of the coupled equations by means of iteration procedure, V and N and V' and N' are unseparated in each order of iteration. *The power series expansion in terms of V or V' alone, therefore, does not correspond to an iterative solution of the basic coupled equation even in its first order expansion.*

It should be born in mind, however, that in the above discussions the

strengths of the interactions were assumed to be variable independently of the wave functions. In particular, V_{np} was treated as if the deuteron could exist in the bound state ϕ_d even in the limit of $V_{np}\to 0$. Actually, however, the wave functions and the interaction potentials are related to each other through Eqs. (2·7) and (2·10). Hence, the discussions given above apply only to the mathematical structure of Eqs. (4·2) and (4·3). In the discussion of the real physical problem interaction potentials should, of course, be kept fixed at the physical values.

§ 5. Summary

A variational principle which makes the S-matrix element stationary was set up and used to derive a set of coupled integro-differential equations for the wave functions describing the (d, d), (d, p), (p, d) and (p, p) reactions in which the d- and p-channels are coupled. The equations are different from those of the coupled channels method for the inelastic scattering because of the non-orthogonality of the d- and p-channels. The coupled terms contain derivatives of the unknown functions. This feature will be avoided in the subsequent paper and the equations will be put in the forms which are symmetrical with respect to channels. An exact and simple expression has also been obtained for the error in the calculated S-matrix elements by means of the theory of finite variation. The effect of the eliminated channels were assumed to be partially taken into account by making the potentials appearing in the equations complex and adjustable so that the experiment can be best reproduced by the theory.

It was shown that there are inherent and legitimate ambiguities in defining the channel wave functions, which necessarily induce the ambiguity in the effective Hamiltonian. This was elucidated with the aid of the projection operator method. This non-uniqueness of the wave functions of relative motion is not trivial for rearrangement reaction because of the non-orthogonality of channels. Our variational principle is not affected by the existence of such ambiguities because only the asymptotic conditions are required. The relation between the method of projection operator and the present one was also discussed.

The relation between DWBA and the present method in weak coupling limit may be summarized as follows. DWBA is equivalent to the first-order solution in iteration in which the interaction kernel as a whole is taken as perturbation. This is different from taking the interaction potential alone as perturbation because of the non-orthogonality terms. *Even in the first order in the interaction potential, the solution of the present method does not agree with DWBA* as long as the non-orthogonality terms are retained.

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Appendix

Proof of Eq. (2·35)

We prove for $M=0$, but the arguments that follow are independent of M. Using $(H-E)\Psi_{L0}^{(2)*}=0$ and assuming H to be real, one has

$$\int \Psi_{L0}^{(2)*}(H-E)\Psi_t^{(1)}d\tau=\int\{\Phi_{00}^{A*}\phi_d{}^*Y_{L0}^*R^{-1}u_L{}^{(2)*}+\sum_{l''}[\Phi_{l_n}^{B*},\ Y_{l''}^*]_{L0}r^{-1}v_{l''}^{(2)*}+\psi_L^{(2)*}\}$$
$$\times(H-E)\{\Phi_{00}^A\phi_dY_{L0}R^{-1}u_{Lt}^{(1)}+\sum_{l'}[\Phi_{l_n}^B,\ Y_{l'}]_{L0}r^{-1}v_{l't}^{(1)}+\psi_t{}^{(1)}\}d\tau-(1\leftrightarrow2)$$
$$=\sum_{i,j=1}^{3}J_{ij}\,. \tag{A·1}$$

In Eq. (A·1), $(1\leftrightarrow2)$ signifies the term which is obtained by exchanging the functions before and after the operator $(H-E)$ in the preceding terms. J_{ij} stands for the integral containing the radial wave function of the i-th channel to the left and that of the j-th channel to the right of $H-E$ minus the same integral with $(1\leftrightarrow2)$ where i or $j=1$, 2 and 3 stands, respectively, for the deuteron channel, the proton channel and all the other channels which are not explicitly taken into account in the present discussion.

Now, let us evaluate J_{ij}. We first calculate J_{11} which can be rewritten as

$$J_{11}=-a_d\int\{\Phi_{00}^{A*}\phi_d{}^*Y_{L0}^*R^{-1}u_L{}^{(2)*}\Delta_R|_{np}\Phi_{00}^A\phi_dY_{L0}u_{Lt}^{(1)}d\xi d\boldsymbol{r}_{np}R^2dRd\hat{\boldsymbol{R}}+a_d(1\leftrightarrow2)$$
$$=-a_d\int\left\{u_L{}^{(2)*}\frac{d^2}{dR^2}u_{Lt}^{(1)}-u_{Lt}^{(1)}\frac{d^2}{dR^2}u_L{}^{(2)*}\right\}dR\,.$$

Carrying out the integration and using (2·30) and (2·31), one gets

$$J_{11}=-a_d(\zeta_L^d)^2T_{dL,pl}^{(L)}\left\{H_L{}^{(+)}(k_d,\ R)\frac{d}{dR}[F_L(k_d,\ R)+T_{dL,dL,t}^{(L)}H_L{}^{(+)}(k_d,R)]\right.$$
$$\left.-[F_L(k_d,\ R)+T_{dL,dL,t}^{(L)}H_L{}^{(+)}(k_d,\ R)]\frac{d}{dR}H_L{}^{(+)}(k_d,\ R)\right\}\Big|_{R\to\infty}$$
$$=-k_da_d(\zeta_L^d)^2T_{dL,pl}^{(L)}\,. \tag{A·2}$$

Next, let us calculate J_{12},

$$J_{12}=-a_p\int\left\{\Phi_{00}^{A*}\phi_d{}^*(\boldsymbol{r}_{np})Y_{L0}^*(\hat{\boldsymbol{R}})R^{-1}u_L{}^{(2)*}(R)\Delta_r|_n\right.$$
$$\left.\times\sum_{l'}[\Phi_{l_n}^B(\xi,\ \boldsymbol{r}_n),\ Y_{l'}(\hat{\boldsymbol{r}})]_{L0}r^{-1}v_{l't}^{(1)}(r)\right\}d\tau+a_p(1\leftrightarrow2)\,. \tag{A·3}$$

Using ϕ_{l_n} defined by (2·9), one can rewrite the right-hand side of (A·3) as

$$J_{12}=-a_p\int\Big\{\phi_d^*\Big(\frac{A}{A+1}\boldsymbol{r}_n-\boldsymbol{r}\Big)Y_{L0}^*(\hat{\boldsymbol{R}})R^{-1}u_L^{(2)*}(R)\Delta_r|_n\sum_{l'}[\phi_{l_n}(\boldsymbol{r}_n),\ Y_{l'}(\hat{\boldsymbol{r}})]_{L0}r^{-1}v_{l'l}^{(1)}(r)$$

$$-\sum_{l'}[\phi_{l_n}(\boldsymbol{r}_n),\ Y_{l'}(\hat{\boldsymbol{r}})]_{L0}r^{-1}v_{l'l}^{(1)}(r)\Delta_r|_n\phi_d^*\Big(\frac{A}{A+1}\boldsymbol{r}_n-\boldsymbol{r}\Big)Y_{L0}^*(\hat{\boldsymbol{R}})R^{-1}u_L^{(2)*}(R)\Big\}\,d\boldsymbol{r}_n r^2 d\boldsymbol{r}d\hat{\boldsymbol{r}}\ , \tag{A·4}$$

which can be transformed into a surface integral by Green's theorem. Since, however, the product $\phi_d^*\phi_{l_n}$ vanishes for very large values of r, the surface integral at infinity vanishes. Hence $J_{12}=0$. Similarly, J_{21} can be shown to be zero. One can also show by a similar argument that $J_{3j}=J_{i3}=0$ for all values of i and j. Only remaining integral is, therefore, J_{22} which can be calculated as

$$J_{22}=\int\{\sum_{l''}[\Phi_{l_n}^{B*},\ Y_{l''}^*]_{L0}r^{-1}v_{l''}^{(2)*}(H-E)\sum_{l'}[\Phi_{l_n}^{B},\ Y_{l'}]_{L0}r^{-1}v_{l'i}^{(1)}\}\,d\hat{\boldsymbol{r}}r^2drd\boldsymbol{r}_n d\xi-(1\leftrightarrow 2)$$

$$=-a_p\int\{\sum_{l''}[\Phi_{l_n}^{B*},\ Y_{l''}^*]_{L0}r^{-1}v_{l''}^{(2)*}\Delta_r|_n\sum_{l'}[\Phi_{l_n}^{B},\ Y_{l'}]_{L0}r^{-1}v_{l'i}^{(1)}\}\,d\hat{\boldsymbol{r}}r^2drd\boldsymbol{r}_n d\xi+a_p(1\leftrightarrow 2)$$

$$=-a_p\sum_{l'}\int\Big\{v_{l'}^{(2)*}\frac{d^2}{dr^2}v_{l'i}^{(1)}-v_{l'i}^{(1)}\frac{d^2}{dr^2}v_{l'}^{(2)*}\Big\}dr$$

$$=-a_p\sum_{l'}(\zeta_{l'}^{p})^2T_{pl',dL,i}^{(L)}\{[F_{l'}(k_p,\ r)\delta_{ll'}+T_{pl',pl}^{(L)*}H_{l'}^{(+)}(k_p,\ r)]\frac{d}{dr}H_{l'}^{(+)}(k_p,\ r)$$

$$-H_{l'}^{(+)}(k_p,\ r)\frac{d}{dr}[F_{l'}(k_p,\ r)\delta_{ll'}+T_{pl',pl}^{(L)*}H_{l'}^{(+)}(k_p,\ r)]\}\,|_{r\to\infty}$$

$$=k_pa_p(\zeta_l^{p})^2T_{pl',dL,i}^{(L)}\ . \tag{A·5}$$

Inserting (A·2) and (A·5) into (A·1), one gets

$$\int\Psi_{L0}^{(2)*}(H-E)\Psi_i^{(1)}d\tau=k_pa_p(\zeta_l^{p})^2T_{pl,dL,i}^{(L)}-k_da_d(\zeta_L^{d})^2T_{dL,pl}^{(L)}\ . \tag{A·6}$$

since all J_{ij} are zero except J_{11} and J_{22}.

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