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Formulation of n-d Elastic and Breakup Reactions
in Terms of the Faddeev Equation with a Local Potential

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We present a heuristic description of a practical theory of n-d elastic and breakup reactions. This is a new version of our three-body theory based on the Faddeev equation with a local potential in coordinate space. We reformulate our previous treatment as legible as possible, and made the following revisions: (i) The structure of the theory is centered on the elastic part of the Faddeev wave function. The breakup components are deduced as necessary ingredients of the elastic part. (ii) Since elastic channel must contain all possible spectator partial waves, it is treated in terms of a multi-channel coupled equation. (iii) Breakup processes to two-body partial waves other than 1S_0 are treated as the perturbation. (iv) The logarithmic singularities in the Faddeev Kernel in the breakup channel are studied in detail, and a practical method of solving our key equation is suggested based on the knowledge of the singularity structure of the solution.

The presentation is detailed enough so that the formulas can immediately be transcribed to suit actual coding of a computational program.

Keywords: n-d elastic and breakup reactions. Faddeev equation.
Local potential.

§1. Introduction

Even after twenty years of pioneering works on the so called Faddeev

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theory on the three-body scattering^{1,2)}, a method and its code for computation of nuclear reaction that is accessible, or at least in its outlook accessible, to conventional nuclear reaction theorists is not available as yet. By outlook, we mean that the theory must be presented in the coordinate space for a local potential, and should be handled as a coupled channel (ordinary differential) equations. The difficulties which we should surmount concerns the treatment of breakup reactions. Under a two-body interaction, one particle is left free, yet the reactions must take place in a finite spacial region. This statement causes a difficulty in the theoretical treatment of the breakup process: In what manner the first half of the sentence is related to the second half? The answer was given by the Faddeev theory: The equation should be written in a manner that the interaction between a pair of particles should follow the interaction between another pair of particles, so that no particle be immune from any collision. Here we should remark that this recipe is not only for theorists, but also for experimentalists, because the quasi-free scattering peak is a manifestation of such a process.

Unfortunately, Faddeev being a mathematician, his theory become understood only after a number of reiterating articles written by physicists. However, even now some nuclear theorists are reluctant to study it presumably because the Faddeev theory is written in momentum space.

With this background, we have strived for constructing a three-body theory of scattering based on the Faddeev equation. We have formulated a theory involving a number of essential ingredients to make the description physical as well as the computation feasible. Also we have proposed techniques by which we can handle parts of the whole theory efficiently. Let us write what we have innovated.

[A] Fundamental concepts

The contributions from poles such as the bound state, virtual state and resonances of subsystems cause physically important effect. Therefore, the theory should be presented in a form that such effects are clearly be seen. On the other hand, once these pole contributions are accommodated properly, the remainder may be handled as the perturbation. Of course, the usual perturbation theory written in a text book of quantum mechanics can not be used for this purpose and we have to construct a new perturbation theory for this purpose. In our opinion, the use of a complete set of functions, such as a complete set of Sturm functions, for calculating a physical quantity is a mathematical illusion of the past time. At a computer age, we should not recourse to it, because any complete set of functions can not be calculated by a computer. The increase of nodes causes the increase of error. As a result, we are forced to truncate, or rather correctly, we have to abandon the calculation without reaching a true value. Thus we prefer the

perturbational treatment. The calculation of a large number of small effects is much easier in the perturbational treatment than otherwise. Based on the same considerations, we have treated three-body bound states by a perturbational approach³⁻⁶⁾.

[B] Fundamental technique

Before any calculation, we know the asymptotic behavior of the wave function of each channel analytically and its behavior near the origin as regular. Therefore, by letting the δ -function singularity of the Green's function involve in the asymptotic behavior, we can construct a compact Green's function for each channel that vanishes at the origin as well as at the asymptotic region. By using this green's function we don't need introducing any artificially boundary, inside of which the breakup reactions are supposed to take place.

[C] Other techniques

(1) Method of continued fraction (MCF) as a method of calculating a scattering problem for a non-local potential⁷⁾: The particle exchange is a characteristic feature of the Faddeev equation, and not only elastic scattering but also all kind of three-body scattering processes are represented as a scattering from a non-local potential. For handling this problem, we have proposed three methods in the past⁸⁻¹⁰⁾, and at last reached the MCF as the most efficient one. This method solves a scattering equation without recourse to any form of perturbational expansion.

(2) Method of acceleration¹⁰⁾: We proposed a method of acceleration for promoting the convergence of a perturbational series. By using this method, we get a convergent value quickly before the error accumulates. After having MCF, the method of acceleration may be used as supplementary; for example, to check the result of MCF. However, the method of acceleration is yet useful especially many states (partial waves or channels) are coupled, in which case the MCF becomes complicated.

(3) Method of partially separable t-matrix CPST¹¹⁾: The effect of the virtual state for the two nucleon 1S_0 state is very important in the n-d scattering. We have introduced an expression in which the effect of this pole is given by a separable term. The remainder does not involve any pole contribution, and may be treated as the perturbation. The separable potential can naturally accommodate the virtual state. Since we do not recourse to the separable potential, we had to introduce the PST.

Our three-body scattering theory based on the Faddeev equation is a result of works over many years³⁻¹⁴⁾. The present paper is intended to be a consistent and unified manual of our theory, together with a collection of necessary techniques^{7,10,11)}. Here, we reformulate reference 14 in a manner that it allows us to represent processes by diagrams, giving a primary role to

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the elastic component. This component will be treated in terms of a multi-channel formalism. Also, the two-body breakup states other than 1S_0 and $^3S_1 + ^3D_1$ states are treated as the perturbation.

Our equation expressed as an integral equation on the real spectator momentum naturally contains the Faddeev kernel much studied by people working in the momentum space representation. It has the well-known logarithmic singularities in the breakup region. In order to determine the method of solving the equation, we must know the singularity structure of terms involved. Following Larson and Hetherington, we investigate these terms and conclude that the solution to our equation is analytic along the real axis of the spectator momentum except for a square-root branch point corresponding to the physical two-body threshold. This enables us to discuss a practical method of solving the equation.

In section 2, we present the antisymmetrized Faddeev equation for n-d elastic and breakup reactions. Some notations used in the later sections are defined. The decomposition of a Faddeev component into elastic and non-elastic components are explained in section 3. An operator Γ is defined which contains all effects other than the elastic channel and which plays a central role in later sections. The elastic wave function $|F\rangle$ is subject to a non-local potential matrix U . An integral equation for the elastic wave is given in a multi-channel formalism. In section 4, we discuss the asymptotic behavior of $|F\rangle$ and define the T and S matrices in the elastic channel. Section 5 deals with the crucial operator Γ which is decomposed into a sum of a non-perturbative part I and a perturbative part W . The non-perturbative part I consists of the contribution of the 1S_0 virtual state pole expressed in a one-term separable form for the absolute value of momentum q less than a judiciously chosen value \bar{q} in the closed channel region and for all real positive q for the breakup region. This is achieved by means of the PST formalism¹¹⁾. The perturbative part W represents the remainder. Both in the non-local potential U in the elastic channel and in the computation of the breakup amplitudes, the operator of a form $(1-\Gamma Q)^{-1}$ appears. Here, Q is the particle exchange operator characteristic to the Faddeev equation. We discuss this operator $(1-\Gamma Q)^{-1}$ using the decomposition of Γ into $I+W$, and derive the fundamental equation expressed as an integral equation over real spectator momentum with the Faddeev kernel. The perturbative treatment of the operator $(1-WQ)^{-1}$ is also presented. This part yields the breakup components of the $^3S_1 + ^3D_1$ and higher partial waves. In section 6, we connect these breakup components in the Faddeev wave function to its asymptotic form and obtain the expression for the breakup amplitudes. In section 7, we present concluding remarks.

Details of various tools used are presented in a number of Appendices. In Appendix A, the PST formalism is reviewed briefly. The presentation for a

coupled two-body states in our previous paper¹¹⁾ needs some revision as discussed here. Appendix B explains how to deal with the perturbative term W near the deuteron pole. In Appendices C and D, we present the formulas to compute the particle exchange operation Q . Appendix C is given for the case with free spectator wave functions, for which the Faddeev kernel with the logarithmic singularities appears. Appendix D deals with formulas for the Q operation when the initial spectator wave function is not free but is under a distorting interaction. The method of solving the elastic channel integral equation is explained in Appendix E. The operation of W requires the computation of operators $(\omega-1)$ and GV . This is explained in Appendix F. The singularity structure of our key integral equation obtained in section 3 is studied in Appendix G. Finally, the method of acceleration is recapitulated.

§2. Faddeev Equation

In this section, we give the antisymmetrized form of the Faddeev equation, and define a number of symbols that are used in later sections.

To begin with, let us forget the antisymmetrization for a moment. Let us denote by $\psi^{(1)}$ the total wave function that has developed from the incident wave $f(1)$ with the deuteron pair (2,3) and the free spectator 1. $\psi^{(1)}$ is decomposed into three Faddeev components.

$$\psi^{(1)} = \phi_1^{(1)} + \phi_2^{(1)} + \phi_3^{(1)} \quad (2.1)$$

For example, the function $\phi_2^{(1)}$ denotes a sum of all possible diagrams in which the last interaction takes place between pair (3,1). This is expressed in the following Faddeev equation.

$$\phi_j^{(\ell)} = f(\ell) \delta_{\ell,j} + G_0 t_j Q \phi_j^{(\ell)} \quad (j=1,2,3) \quad (2.2)$$

We have introduced the particle exchange operator Q by

$$Q \phi_j^{(\ell)} = \phi_k^{(\ell)} + \phi_i^{(\ell)} \quad (i,j,k \text{ cyclic}) \quad (2.3)$$

Now, we antisymmetrize the total wave function by taking the combination

$$\Psi = \frac{1}{\sqrt{3}} (\psi^{(1)} + \psi^{(2)} + \psi^{(3)}) \quad (2.4)$$

This is totally antisymmetric because (i) in the incident wave $f(i)$, the deuteron pair (j,k) is antisymmetrized, and (ii) the total Hamiltonian is symmetric in particle labels. In this regard, one should remember that Ψ

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satisfies the three-body Schrodinger equation.

Instead of dealing with three equations (2.2) for nine components $\phi_j^{(\ell)}$ with awkward $\delta_{\ell,j}$ in it, we recombine these functions to define

$$\phi_i = \phi_i^{(1)} + \phi_i^{(2)} + \phi_i^{(3)} \quad (i=1,2,3) \quad . \quad (2.5)$$

Then Eqs. (2.2) and (2.4) become

$$\Psi = \frac{1}{\sqrt{3}} (\phi_1 + \phi_2 + \phi_3) \quad (2.6)$$

and

$$\phi_i = f(i) + G_0 t_i Q \phi_i \quad (i=1,2,3) \quad . \quad (2.7)$$

ϕ_i has the incident wave $f(i)$, and also it represents the sum of all diagrams in which the last interaction takes place between pair (j,k) . Since three equations in Eq. (2.7) are equivalent, we only need to solve one of them. From now on, unless necessary, we drop the suffix i in Eq. (2.7) and write it as

$$|\phi\rangle = |f\rangle + G_0 t Q |\phi\rangle \quad . \quad (2.8)$$

In our formulation, we use the following symbols. For the spin-isospin-angular function with the total spin, parity, and isospin $J_0^{\pi} M_0 T M_T$, we use

$$|\alpha(23,1)\rangle = |(LS)J, (\ell \frac{1}{2})j; J_0^{\pi} M_0(23,1)\rangle |I \frac{1}{2}; T M_T(23,1)\rangle \quad . \quad (2.9)$$

Here, L, S, J , and I refer to the pair $(2,3)$ and (ℓj) to the particle 1. For a coupled two-body state, $|\alpha\rangle$ is a 1×2 row vector. In particular, we denote by $|\alpha_0(23,1)\rangle$ the states in which the pair $(2,3)$ is in the ${}^3S_1 + {}^3D_1$ state.

$$|\alpha_0\rangle = |\alpha({}^3S_1, {}^2\ell_j), \alpha({}^3D_1, {}^2\ell_j)\rangle \quad . \quad (2.10)$$

The radial part of the deuteron wave function is referred to as ϕ_d ,

$$|\phi_d\rangle = \begin{pmatrix} |\phi_d({}^3S_1)\rangle \\ |\phi_d({}^3D_1)\rangle \end{pmatrix} \quad . \quad (2.11)$$

The incident wave $f(1)$ is the projection of the product

$$|f(1)\rangle = [\phi_d(23) \cdot e^{i\vec{p}_0 \cdot \vec{Y}_1}]_{j_0^{\pi} M_0, T M_T}$$

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$$= \sum_{\alpha_0} \beta_{\alpha_0} |\alpha_0 \phi_d(x_{23}) \rangle |j_\ell(p_0 y_1) \rangle . \quad (2.12)$$

Here, the sum \sum is taken over all possible (ℓj) for a given $(J_0^\pi M_0, T M_T)$. A constant β_{α_0} is the weight (a product of Clebsch-Gordon coefficients). The function $j_\ell(p_0 y)$ denotes the spherical Bessel function, p_0 being the incident momentum

$$p_0 = \sqrt{\frac{4M}{3\hbar^2} (E + |E_d|)} . \quad (2.13)$$

Throughout the text, we use the notation V for a local two-nucleon potential multiplied by M/\hbar^2 , M being the nucleon mass. Further, we define all Green functions with the factor \hbar^2/M . For example,

$$G_0 = \frac{\hbar^2}{M} \frac{1}{E - H_0 + i\epsilon} \quad (2.14)$$

where H_0 is the sum of kinetic energy operators,

$$H_0 = T_x + T_y . \quad (2.15)$$

We also use the notations $T_L(x)$ and $T_\ell(y)$ for partial wave kinetic energy operators. Thus, for example,

$$G_a = \frac{\hbar^2}{M} \frac{1}{E - T_L(x) - T_\ell(y) - \frac{\hbar^2}{M} V_a + i\epsilon} . \quad (2.16)$$

To deal with the breakup threshold behavior correctly, it is better to introduce following notations for interacting pairs,

$$\hat{j}_L(qx) = j_L(qx)/q^L \quad (2.17)$$

$$\hat{h}_L^{(+)}(qx) = q^{L+1} h_L^{(+)}(qx) \quad (2.18)$$

and

$$\hat{n}_L^{(+)}(qx) = q^{L+1} n_L(qx) . \quad (2.19)$$

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These notations will appear throughout appendices.

§3. Decomposition into Elastic and Non-elastic Components

Since Eq.(2.8) is a linear equation, we can express $|\phi\rangle$ as

$$|\phi\rangle = \sum_{\alpha_0} \beta_0 |\phi_{\alpha_0}\rangle \quad (3.1)$$

Using Eqs.(2.12) and (3.1) in Eq.(2.8), we find the Faddeev equation for $|\phi_{\alpha_0}\rangle$.

$$|\phi_{\alpha_0}\rangle = |\alpha_0\phi_d j_\ell\rangle + GVQ|\phi_{\alpha_0}\rangle \quad (3.2)$$

The suffix α_0 on $|\phi_{\alpha_0}\rangle$ is to indicate its initial component. It has all three-body components that can develop from $|\alpha_0\phi_d j_\ell\rangle$.

On the right-hand side of Eq.(3.2), we insert the identity between G and V,

$$1 = \sum_{\alpha_0} |\alpha_0\phi_d\rangle\langle\phi_d\alpha_0| + [1 - \sum_{\alpha_0} |\alpha_0\phi_d\rangle\langle\phi_d\alpha_0|] \quad (3.3)$$

Thus

$$|\phi_{\alpha_0}\rangle = |\alpha_0\phi_d j_\ell\rangle + \sum_{\alpha'_0} G|\alpha'_0\phi_d\rangle\langle\phi_d\alpha'_0|VQ|\phi_{\alpha_0}\rangle + \Gamma Q|\phi_{\alpha_0}\rangle \quad (3.4)$$

where we have defined the operator Γ by

$$\Gamma = G[1 - \sum_{\alpha_0} |\alpha_0\phi_d\rangle\langle\phi_d\alpha_0|]V \quad (3.5)$$

In Eq.(3.4), we rewrite $G|\alpha'_0\phi_d\rangle$ as follows.

$$\begin{aligned} G|\alpha'_0\phi_d\rangle &= \frac{\hbar^2}{M} \frac{1}{E - T_{\vec{x}} - T_{\vec{y}} - V + i\epsilon} |\alpha'_0\phi_d\rangle = \frac{\hbar^2}{M} \frac{1}{E + |E_d| - T_{\vec{y}} + i\epsilon} |\alpha'_0\phi_d\rangle \\ &= |\alpha'_0\phi_d\rangle \frac{4}{3} \check{G}_{0,\ell} \end{aligned} \quad (3.6)$$

where $\check{G}_{0,\ell}$ is the (partial-wave) Green function for the spectator

$$G_{0,\ell} = \frac{3}{4} \frac{\hbar^2}{M} \frac{1}{E + |E_d| - T_{\vec{y}} + i\epsilon} = \frac{1}{p_0^2 - \frac{4M}{3\hbar^2} T_{\vec{y}} + i\epsilon}$$

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$$= -p_0 [h_\ell^{(+)}(p_0 y) j_\ell(p_0 y') \Theta(y-y') + j_\ell(p_0 y) h_\ell^{(+)}(p_0 y') \Theta(y'-y)] \quad (3.7)$$

Thus, Eq.(3.4) becomes

$$|\phi_{\alpha_0}\rangle = |\alpha_0 \phi_d j_\ell\rangle + \sum_{\alpha'_0} |\alpha'_0 \phi_d\rangle \frac{4}{3} \check{G}_{0,\ell} \langle \phi_d \alpha'_0 | \bar{V} Q | \phi_{\alpha_0}\rangle + \Gamma Q |\phi_{\alpha_0}\rangle \quad (3.8)$$

Let us define the elastic channel wave function $|F_{\alpha'_0 \alpha_0}\rangle$ by

$$|F_{\alpha'_0 \alpha_0}\rangle = \delta_{\alpha'_0 \alpha_0} |j_\ell\rangle + G_{0,\ell} \langle \phi_d \alpha'_0 | \bar{V} Q | \phi_{\alpha_0}\rangle \quad (3.9)$$

with

$$\bar{V} = \frac{4}{3} V \quad (3.10)$$

Then we have from Eq.(3.8)

$$|\phi_{\alpha_0}\rangle = \sum_{\alpha'_0} |\alpha'_0 \phi_d\rangle F_{\alpha'_0 \alpha_0} + \Gamma Q |\phi_{\alpha_0}\rangle \quad (3.11)$$

As we show in Appendix B, Eq.(3.5) defines the operator Γ which is free from the deuteron pole. Therefore, in the asymptotic region it has no elastic components. We postpone the discussion of Γ until Section 5. The solution of Eq.(3.11) is formally expressed as

$$|\phi_{\alpha_0}\rangle = \sum_{\alpha'_0} (1-\Gamma Q)^{-1} |\alpha'_0 \phi_d\rangle F_{\alpha'_0 \alpha_0} \quad (3.12)$$

Substituting this expression for $|\phi_{\alpha_0}\rangle$ on the right-hand side of Eq.(3.9), we obtain

$$|F_{\alpha'_0 \alpha_0}\rangle = \delta_{\alpha'_0 \alpha_0} |j_\ell\rangle + \sum_{\alpha''_0} \check{G}_{0,\ell} U_{\alpha'_0 \alpha''_0} |F_{\alpha''_0 \alpha_0}\rangle \quad (3.13)$$

where we have defined the non-local potential

$$V_{\alpha_0 \alpha'_0} = \langle \alpha_0 \phi_d | \bar{V} Q (1-\Gamma Q)^{-1} | \alpha'_0 \phi_d \rangle \quad (3.14)$$

Eq.(3.13) is a set of coupled integral equations for elastic wave functions.

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The non-local potential $U_{\alpha_0\alpha'_0}$ couples $(\ell'j')$ in $|\alpha'_0\rangle$ to (ℓj) in $|\alpha_0\rangle$ for a given $(J_0^{\pi M_0}, TM_T)$. Eq.(3.13) can be written in a matrix form

$$|F\rangle = |j\rangle + \check{G}_0 U |F\rangle \quad (3.15)$$

where $|j\rangle$ and \check{G}_0 are diagonal. The elastic component can be obtained by solving Eq.(3.15). Then the breakup component can be found from Eq.(3.12). In this course, we need to know how to deal with the operator $(1-\Gamma Q)^{-1}$ in Eq.(3.14). This will be discussed in Sections 5 and 6. Before doing so, let us discuss the asymptotic behavior of $|F\rangle$ in the next section, and define the elastic scattering amplitude.

§4. Elastic Scattering Amplitude

The asymptotic form of the elastic wave function $|F\rangle$ can be found from Eqs.(3.7) and (3.15).

$$|F\rangle \xrightarrow{y \rightarrow \infty} |j\rangle - p_0 |h^{(+)}\rangle \langle j|V|F\rangle \quad (4.1)$$

Here, $|h^{(+)}\rangle$ is diagonal and so is $\langle j|$ and $|j\rangle$. They all refer to all possible (ℓj) in $|\alpha_0\rangle$ for a given $(J_0^{\pi M_0}, TM_T)$. Let us define the T matrix in the elastic channel.

$$T = -p_0 \langle j|U|F\rangle \quad (4.2)$$

Then, we have from Eq.(4.1)

$$|F\rangle \xrightarrow{y \rightarrow \infty} |j\rangle + |h^{(+)}\rangle T = -\frac{1}{2i} [|h^{(-)}\rangle - |h^{(+)}\rangle S] \quad (4.3)$$

where the S matrix in the elastic channel is defined by

$$S = 1 + 2iT \quad (4.4)$$

Let us define the stationary solution $|\xi\rangle$ as the solution to

$$|\xi\rangle = |j\rangle + P\check{G}_0 U |\xi\rangle \quad (4.5)$$

where $P\check{G}_0$ is the principal value Green function.

$$P\check{G}_0 = \check{G}_0 + ip_0 |j\rangle \langle j| \quad (4.6)$$

$$p\tilde{G}_{0,\ell} = p_0 [n_\ell(p_0 y) j_\ell(p_0 y') \Theta(y-y') + j_\ell(p_0 y) n_\ell(p_0 y') \Theta(y'-y)] \quad (4.7)$$

In terms of $|\xi\rangle$, $|F\rangle$ is given by

$$|F\rangle = |\xi\rangle [1+iT] \quad (4.8)$$

The asymptotic form of $|\xi\rangle$ can be found from Eqs.(4.5) and (4.7).

$$|\xi\rangle \xrightarrow{y \rightarrow \infty} |j\rangle - |n>K \quad (4.9)$$

where we have defined the K matrix by

$$K = -p_0 \langle j|V|\xi\rangle \quad (4.10)$$

T, K and S are related as follows.

$$T = (1-iK)^{-1}K \quad (4.11)$$

$$S = (1-iK)^{-1}(1+iK) \quad (4.12)$$

From time-reversal, K must be symmetric. Below breakup threshold, K must be real so that S is unitary.

The elastic component of $|\phi_{\alpha_0}\rangle$ is the first term in the right-hand side of Eq.(3.11). With Eq.(4.3) this becomes

$$|\phi_{\alpha_0}^{\text{Elastic}}\rangle = \sum_{\alpha'_0} |\alpha'_0 \phi_d^F \alpha'_0 \alpha_0\rangle \xrightarrow{y \rightarrow \infty} \sum_{\alpha'_0} |\alpha'_0 \phi_d\rangle [\delta_{\alpha'_0 \alpha_0} |j_\ell\rangle + |h_{\ell'}^{(+)}\rangle T_{\alpha'_0 \alpha_0}] \quad (4.13)$$

Therefore, the elastic component of $|\phi\rangle$ of Eq.(3.1) becomes asymptotically

$$\begin{aligned} |\phi^{\text{Elastic}}\rangle &\xrightarrow{y \rightarrow \infty} \sum_{\alpha_0} \beta_{\alpha_0} \sum_{\alpha'_0} |\alpha'_0 \phi_d\rangle [\delta_{\alpha'_0 \alpha_0} |j_\ell\rangle + |h_{\ell'}^{(+)}\rangle T_{\alpha'_0 \alpha_0}] \\ &= \sum_{\alpha'_0} \beta_{\alpha_0} |\alpha'_0 \phi_d j_\ell\rangle + \sum_{\alpha'_0} |\alpha'_0 \phi_d h_{\ell'}^{(+)}\rangle \sum_{\alpha_0} \beta_{\alpha_0} T_{\alpha'_0 \alpha_0} \end{aligned} \quad (4.14)$$

The first term of this expression is just the incident wave, Eq.(2.12).

Therefore, the elastic scattering amplitude is given by

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$$f^{el}(J_0 \pi M_0, TM_T) = \frac{1}{p_0} \sum_{\alpha'_0} i^{-\ell'} |\alpha'_0\rangle \sum_{\alpha_0} \beta_{\alpha_0} T_{\alpha'_0 \alpha_0} \quad (4.15)$$

where, we have used $|h_{\ell'}^{(+)}\rangle \xrightarrow{y \rightarrow \infty} e^{i(p_0 y - \frac{\ell'}{2}\pi)} / p_0 y$.

This amplitude is for partition (23,1). Although the total wave function Ψ is given by Eq.(2.6), in the asymptotic region the elastic components of ϕ_1, ϕ_2 and ϕ_3 do not overlap. Therefore the elastic scattering cross section is simply given by

$$d\sigma^{el}(J_0 \pi M_0, TM_T) = |f^{el}(J_0 \pi M_0, TM_T)|^2 \quad (4.16)$$

To conclude this section, let us write out how to calculate the phase shifts. Let u_k be the eigenvector of the K matrix with an eigenvalue κ_k .

$$K u_k = \kappa_k u_k \quad (k=1, 2, \dots, N) \quad (4.17)$$

If there are N possible (ℓj) in $|\alpha_0\rangle$ with $(J_0 \pi M_0, TM_T)$, then u_k is a $(N \times 1)$ row vector. Let ω be the $N \times N$ matrix composed of u_k ($k=1$ to N).

$$\omega = (u_1, u_2, \dots, u_N) \quad (4.18)$$

Further, let κ be the diagonal matrix whose diagonal elements are κ_k . Then Eq.(4.14) can be written as

$$K\omega = \omega\kappa \quad (4.19)$$

To Eq.(4.12), we multiply ω from the right and the transpose of ω from the left.

$$\omega^T S \omega = (1-i\kappa)^{-1} \omega^T \omega (1+i\kappa) \quad (4.20)$$

Since K is symmetric, ω is orthogonal. This means $\omega^T = \omega^{-1}$. Therefore, we see that S is diagonalized by ω :

$$\omega^{-1} S \omega = \frac{1+i\kappa}{1-i\kappa} = e^{2i\delta} \quad (4.21)$$

which defines the phase shift δ (a diagonal matrix). Below the breakup threshold it is real. Above the breakup threshold δ becomes complex ($I_m \kappa > 0$ is required).

§5. Operator Γ and the Key Equation

Hereafter, we shall often suppress the state label α whenever possible, and write Eqs.(3.11) and (3.12) simply as

$$|\phi\rangle = |\phi_d F\rangle + \Gamma Q |\phi\rangle \quad (5.1)$$

and

$$|\phi\rangle = (1-\Gamma Q)^{-1} |\phi_d F\rangle \quad (5.2)$$

To obtain $|F\rangle$, we solve Eq.(4.5).

$$|\xi\rangle = |j\rangle + P G_0 \langle \phi_d | \bar{V} Q (1-\Gamma Q)^{-1} | \phi_d \xi \rangle \quad (5.3)$$

The asymptotic form of Eq.(5.3) yields the K-matrix of Eq.(4.10), in terms of which the elastic T-matrix is given by Eq.(4.11). Thus we can calculate $|F\rangle$ by Eq.(4.8).

$$|F\rangle = |\xi\rangle (1+iT). \quad (5.4)$$

To solve Eq.(5.3), we use the iterative scheme of Horacek and Sasakawa⁷⁾. As is explained in Appendix E, during the process of iterative solutions, we need to operate the non-local potential V of Eq.(3.14) on the i th iterate $|f^{(1)}\rangle$ as in Eq.(E.14). Therefore the operator $(1-\Gamma Q)^{-1}$ in V need be operated on a known function $|\phi_d f^{(1)}\rangle$.

We could conceive an alternative method of solving Eq.(5.3) in which it is expressed as a set of coupled equations among expansion coefficients of $|\xi\rangle$ in terms of, say, the spherical Bessel functions. Then we can solve this set of equations by a matrix inversion. There again, the operator $(1-\Gamma Q)^{-1}$ operates on known functions.

After having solved Eq.(5.3), we compute $|F\rangle$ by Eq.(5.4), and then $|\phi\rangle$ by Eq.(5.2). However, this last step is in fact unnecessary. In solving Eq.(5.3), we have already computed $(1-\Gamma Q)^{-1} |\phi_d \xi\rangle$.

In any case, what we need to know is how to operate $(1-\Gamma Q)^{-1}$ on a function $|\phi_d \chi\rangle$ where $|\chi\rangle$ is a given function of y .

Therefore, let us define

$$|\rho\rangle = (1-\Gamma Q)^{-1} |\phi_d \chi\rangle \quad (5.5)$$

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The integral equation for $|\rho\rangle$ is

$$|\rho\rangle = |\phi_d\rangle + \Gamma Q|\rho\rangle \quad (5.6)$$

Now, we come to a point where we must decide how to treat Γ . First of all, we must expand Γ into partial waves. Introducing the complete set of orthonormalized functions $|F_\alpha\rangle$ by

$$|F_\alpha\rangle = |\alpha \cdot u_\alpha\rangle = |\alpha \cdot u_\alpha(p, y)\rangle = |\alpha \cdot \sqrt{\frac{2}{\pi}} p j_\ell(py)\rangle \quad (5.7)$$

we find from Eq. (3.5)

$$\Gamma = \sum_\alpha |F_\alpha\rangle G_\alpha \langle F_\alpha| [1 - \sum_{\alpha_0} |\alpha_0 \phi_d\rangle \langle \phi_d \alpha_0|] V \quad (5.8)$$

where $\sum_\alpha = \sum_\alpha \int_0^\infty dp$, and

$$\begin{aligned} G_\alpha &= \frac{\hbar^2}{M} [E - \frac{3\hbar^2}{4M} p^2 - T_L(x) - \frac{\hbar^2}{M} V + i\varepsilon]^{-1} \\ &= [q^2 - \frac{M}{\hbar^2} T_L(x) - V + i\varepsilon]^{-1} \end{aligned} \quad (5.9)$$

The momentum q of the interacting pair is defined by

$$\frac{\hbar^2}{M} q^2 = E - \frac{3\hbar^2}{4M} p^2 \quad (5.10)$$

For $E < 0$ (below breakup threshold), $q = i|q|$. Since the deuteron pole is extracted out in Eq. (5.8), there remain only closed channels for $E < 0$. For $E > 0$ and $0 < p < p_c = \sqrt{4ME/3\hbar^2}$, q is real positive. This is the breakup region, although there are some closed channel components as we shall see. For $E > 0$ and $p > p_c$, again $q = i|q|$ and this belongs to the closed channel region.

The operator Γ has all the effects of breakup and closed channels except the deuteron pole. Among others, the 1S_0 virtual state pole has the strongest effect and should be treated as an unperturbed part. The effect of the $^3S_1 + ^3D_1$ state, on the other hand, may very well be treated by perturbation, since the deuteron pole has already been extracted out. All higher partial waves may also be treated as perturbation. Thus we split Γ into the 1S_0 pole term I and the rest W . The unperturbed part I is given by the separable pole term of the PST decomposition of $G_0 t(^1S_0)$ (See Appendix A) for p less than a judiciously chosen value \bar{p} . The perturbation W represents all the remainder. Thus Γ takes the form

$$\Gamma = \sum_{\alpha}^{(I)} |F_{\alpha}^U \rangle \langle \tau_{\alpha} F_{\alpha} | + \sum_{\alpha}^{(W)} |F_{\alpha} \rangle W_{\alpha} (F_{\alpha} | \quad . \quad (5.11)$$

The functions $|U_{\alpha}\rangle$ and $\langle \tau_{\alpha} |$ are given in Table 1, and the operator W_{α} in Table 2. For $|\alpha\rangle$ with the ${}^3S_1 + {}^3D_1$ two-body state, W_{α} requires a special treatment for q near iq_d ($q_d = \sqrt{M|E_d|}/\hbar$). See Appendix B for the details. The calculation of $(\omega-1)$ and GV in W_{α} is discussed in Appendix F.

Before proceeding any further, let us draw schematic diagrams of the treatment so far. We shall represent $G_0 t$ by the diagram of Fig. 1. The Faddeev equation (2.8) is depicted in Fig. 2. We shall represent Γ by a spring in Fig. 3. Then, the extraction of the deuteron pole from $G_0 t$ would be given by Fig. 4. In Fig. 5, we illustrate the elastic component $|F\rangle$ of Eq.(3.9). Then Eq.(5.1) for $|\phi\rangle$ is given by Fig. 6. The decomposition (5.11) of Γ is represented as Fig. 7.

Let us simply write Eq.(5.11) as

$$\Gamma = |FU\rangle \langle \tau F| + W, \quad (5.12)$$

where the summation symbol \sum_{α} has been suppressed.

On substituting this expression of Γ into Eq.(5.6) and treating W as perturbation, we find

$$|\rho\rangle = (1-WQ)^{-1} |\phi_d \chi\rangle + (1-WQ)^{-1} |FU\rangle A \quad (5.13)$$

where

$$A = \langle \tau F | Q | \rho \rangle \quad . \quad (5.14)$$

Multiplying $\langle \tau F | Q |$ to Eq.(5.13) from the left, we obtain our key equation

$$M = M + NA, \quad (5.15)$$

where we have defined

$$M = \langle \tau F | Q (1-WQ)^{-1} | \phi_d \chi \rangle \quad (5.16)$$

and

$$N = \langle \tau F | Q (1-WQ)^{-1} | FU \rangle \quad (5.17)$$

The perturbation expansion of $(1-WQ)^{-1}$ is illustrated in Fig. 8. If $|\rho\rangle$ is

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depicted by the same diagram as $|\phi\rangle$ (see Fig. 6), then A can be pictured as in Fig. 9. For M and N, we have diagrams of Figs. 10 and 11. Finally, the diagrammatic representation of Eq.(5.13) is given by Fig. 12.

The zero-th order term of M is $\langle \tau F | Q | \phi_d \chi \rangle$. Since $|\chi\rangle$ here is either the i th iteration $|\xi^{(i)}\rangle$ to Eq.(5.3) or $|F\rangle$ in Eq.(5.2), it is not a plane wave but a distorted spectator function. Therefore to compute $\langle \tau F | Q | \phi_d \chi \rangle$, we need the method developed in refs. 4 and 6 for distorted spectator functions (see Appendix D). For the first and higher order M and for all orders of N, the matrix elements are all of the form $\langle \tau_{\alpha} F_{\alpha} | Q | F_{\alpha}, Z_{\alpha}, (x) \rangle$. Specifically, we define

$$|\eta_{\alpha}(x)\rangle = \sum_{m=1}^{\infty} |\eta_{\alpha}^{(m)}(x)\rangle \quad (5.18)$$

with

$$|\eta_{\alpha}^{(1)}(x)\rangle = (F_{\alpha} | Q | \alpha_0 \phi_d \chi \rangle \quad \text{for M} \quad (5.19a)$$

$$= (F_{\alpha} | Q | F_{\alpha}, Z_{\alpha}, \rangle \quad \text{for N} \quad (5.19b)$$

and

$$|\eta_{\alpha}^{(m)}(x)\rangle = S_{\alpha}^{(w)} (F_{\alpha} | Q | F_{\alpha}, Z_{\alpha}^{(m)}(x) \rangle \quad (m \geq 2) \quad (5.20)$$

where

$$|Z_{\alpha}^{(m)}(x)\rangle = W_{\alpha} |\eta_{\alpha}^{(m-1)}(x)\rangle \quad (m \geq 2) \quad (5.21)$$

Then M_{α} and $N_{\alpha\alpha}$ are given by $\langle \tau_{\alpha} | \eta_{\alpha} \rangle$ (notice that $|\eta_{\alpha}\rangle$ are different for M and N). The calculation of $(F_{\alpha} | Q | F_{\alpha}, Z_{\alpha}, \rangle$ is best treated by the method described in ref. 18 for plane wave spectator functions (see Appendix C). As a function of p and p' along the real (positive) axis, $(F_{\alpha} | Q | F_{\alpha}, Z_{\alpha}, \rangle$ has logarithmic singularities (see Appendix C). The method of solving our key equation, Eq. (5.15), depends essentially on the analytic property of the solution vector $A_{\alpha}(p)$ as a function of p along the real axis. This is investigated in Appendix G using the technique of Larson and Hetherington²²). There, it is shown that $A_{\alpha}(p)$ is an analytic function of p except for a square-root branch point at the breakup threshold $p=p_c$, and it goes to zero as $p \rightarrow 0$. Based on this knowledge, we employ the method proposed in ref. 9 to solve Eq.(5.15) in the following manner. Let us divide the entire p interval into four regions.

$$\begin{array}{ll}
\text{Region I} & 0 < p < \sqrt{ME/h^2} \\
\text{Region II} & \sqrt{ME/h^2} < p < p_c \quad (= \sqrt{4ME/3h^2}) \\
\text{Region III} & p_c < p < \bar{p} \\
\text{Region IV} & \bar{p} < p < \infty
\end{array} \tag{5.22}$$

(For \bar{p} , see Tables 1 and 2.) For each region, we choose appropriate "standard" mesh points and an appropriate interpolation function $\mathcal{L}_i(p)$ (e.g., Lagrange interpolation function) to interpolate $A_\alpha(p)$ by

$$A_\alpha(p) = \sum_i \mathcal{L}_i(p) A_\alpha(p_i) \tag{5.23}$$

The summation runs over the standard mesh points within the region to which p_i belongs, not over the entire mesh points. With the conditions on $\mathcal{L}_i(p)$

$$\mathcal{L}_i(p_j) = \delta_{i,j} \quad ; \quad \mathcal{L}_i(0) = 0 \tag{5.24}$$

Eq.(5.15) becomes

$$A_\alpha(p_i) = M_\alpha(p_i) + \sum_\beta \sum_j \Omega(\alpha i, \beta j) A_\beta(p_j) \tag{5.25}$$

with

$$\Omega(\alpha i, \beta j) = \int dp' N(\alpha p_i, \beta p') \mathcal{L}_j(p') \tag{5.26}$$

The p' integral here is over the region to which p_j belongs, not over the entire p interval. The summation \sum_j in Eq.(5.25) now runs over the entire standard mesh points. To deal with the square-root branch point correctly, in Region II and Region III we employ the integration variable q'

$$\begin{array}{ll}
q' = \sqrt{p_c^2 - p'^2} & \text{for Region II} \\
|q'| = \sqrt{p'^2 - p_c^2} & \text{for Region III,}
\end{array} \tag{5.27}$$

with an appropriate $\mathcal{L}_i(q')$ and with judiciously chosen secondary q' mesh points to carry out the q' integration rather than the p' integration in Eq.(5.26). In Region I, we may use the standard p mesh for the p' integration.

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Although $A_\alpha(p)$ exists only over $0 \leq p < \bar{p}$, the p' integration in Eq.(5.26) runs over Region IV also. Here we introduce a variable Z by

$$p' = \bar{p} + \frac{Zs}{1-Z}, \quad 0 \leq Z < 1 \quad (5.28)$$

with a parameter s , and set up secondary Z mesh points and a suitable $\mathcal{L}_i(Z)$ to carry out the Z -integration.

The advantage of the above method of solving Eq.(5.15) is clear. The complicated p' integration involving the singular kernel is decoupled from Eq.(5.25). The matrix elements $\Omega(\alpha_i, \beta_j)$ can be calculated in advance with sufficient accuracy to be used over and over again, while Eq.(5.25) can be solved by a matrix inversion. This will speed up considerably the solution of Eq.(5.3) by iteration during which $(1-\Gamma Q)^{-1} |\phi_d \xi^{(i)}\rangle$ must be calculated many times.

§6. The Total Wave Function and Breakup Amplitudes

The Faddeev component $|\phi_{\alpha_0}\rangle$ of Eq.(3.12) can be expressed in the form of Eq.(5.13).

$$|\phi_{\alpha_0}\rangle = \sum_{\alpha'_0} [(1-WQ)^{-1} |\alpha'_0 \phi_d^F \alpha'_0 \alpha_0\rangle + (1-WQ)^{-1} S_{\alpha}^{(I)} |F_{\alpha} \cup_{\alpha} \rangle A_{\alpha}^{\alpha_0 \alpha_0}] \quad (6.1)$$

where

$$A_{\alpha}^{\alpha_0 \alpha_0} = \langle \tau_{\alpha}^F | Q | \alpha'_0 \phi_d^F \alpha'_0 \alpha_0 \rangle \quad (6.2)$$

We shall suppress all indices referring to α_0 and α'_0 in this section. The amplitude A_{α} can be obtained by solving, as explained in section 6,

$$A_{\alpha} = M_{\alpha} + S_{\alpha'}^{(I)} N_{\alpha \alpha'} A_{\alpha'} \quad (6.3)$$

with M_{α} and $N_{\alpha \alpha'}$ defined by Eqs.(5.16) and (5.17) with $|\chi\rangle = |F\rangle$. Treating $(1-WQ)^{-1}$ as the perturbation, we find

$$(1-WQ)^{-1} |\phi_d^F\rangle = |\phi_d^F\rangle + S_{\alpha'}^{(w)} |F_{\alpha'} \rangle W_{\alpha'} | \eta_{\alpha'} \rangle (x) \quad (6.4)$$

where

$$|\eta_{\alpha'} \rangle (x) = \sum_{m=1}^{\infty} |\eta_{\alpha'}^{(m)} \rangle (x) \quad (6.5)$$

with

$$|\eta_{\alpha'}^{(1)}(x)\rangle = (F_{\alpha'}, |Q|\phi_d^F\rangle \quad (6.6)$$

$$|\eta_{\alpha'}^{(m)}(x)\rangle = S_{\alpha''} (F_{\alpha'}, |Q|F_{\alpha''} z_{\alpha''}^{(m)}(x)\rangle \quad (m \geq 2) \quad (6.7)$$

and

$$|z_{\alpha''}^{(m)}(x)\rangle = W_{\alpha''} |\eta_{\alpha''}^{(m-1)}(x)\rangle \quad (m \geq 2)$$

Similarly,

$$(1-WQ)^{-1} |F_{\alpha'}^U\rangle = |F_{\alpha'}^U\rangle + S_{\alpha'}^{(w)} |F_{\alpha'}\rangle W_{\alpha'} |\zeta_{\alpha'}(x)\rangle \quad (6.9)$$

where

$$|\zeta_{\alpha'}(x)\rangle = \sum_{m=1}^{\infty} |\zeta_{\alpha'}^{(m)}(x)\rangle \quad (6.10)$$

with

$$|\zeta_{\alpha'}^{(1)}(x)\rangle = (F_{\alpha'}, |Q|F_{\alpha'}^U\rangle \quad (6.11)$$

$$|\zeta_{\alpha'}^{(m)}(x)\rangle = S_{\alpha''} (F_{\alpha'}, |Q|F_{\alpha''} z_{\alpha''}^{(m)}(x)\rangle \quad (m \geq 2) \quad (6.12)$$

and

$$|z_{\alpha''}^{(m)}(x)\rangle = W_{\alpha''} |\zeta_{\alpha''}^{(m-1)}(x)\rangle \quad (m \geq 2) \quad (6.13)$$

With Eqs. (6.3) and (6.8), Eq. (6-1) becomes

$$|\phi\rangle = |\phi_d^F\rangle + S_{\alpha'}^{(I)} |F_{\alpha'}^U\rangle A_{\alpha'} + S_{\alpha'}^{(w)} |F_{\alpha'}\rangle W_{\alpha'} |\psi_{\alpha'}(x)\rangle \quad (6.14)$$

where

$$|\psi_{\alpha'}(x)\rangle = |\eta_{\alpha'}(x)\rangle + S_{\alpha'}^{(I)} |\zeta_{\alpha'}(x)\rangle A_{\alpha'} \quad (6.15)$$

The first term on the right-hand side of Eq. (6.14) is the elastic component

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of $|\phi\rangle$. The second and the third terms represent the non-elastic component. They yield breakup components at asymptotic region. The asymptotic form of the second term of Eq.(6.14) is given by the 1S_0 component

$$|F_{\alpha} \cup_{\alpha} \rangle A_{\alpha} = -|F_{\alpha} \omega_{\alpha} \hat{\phi}_{\alpha} \rangle A_{\alpha} \xrightarrow{x \rightarrow R} -|F_{\alpha} \cdot \hat{h}_L^{(+)}(qx) \rangle A_{\alpha} \quad (6.16)$$

($|\alpha\rangle = |\alpha(^1S_0)\rangle$ here) where we have used Eqs.(5.7), (A.1), (A.5) and (A.21). The asymptotic form of the third term of Eq.(6.14) comes from the operator GV in the $^3S_1 + ^3D_1$ and higher partial waves in the positive energy region of W_{α} in Table 2.

$$|F_{\alpha} \rangle W_{\alpha} |\psi_{\alpha}(x)\rangle \xrightarrow{x \rightarrow \infty} |F_{\alpha} \rangle G_{\alpha} U_a |\psi_{\alpha}(x)\rangle \xrightarrow{x \rightarrow \infty} |F_{\alpha} \cdot \hat{h}_L^{(+)}(qx) \rangle C_{\alpha} \quad (6.17)$$

($|\alpha\rangle \neq |\alpha(^1S_0)\rangle$ here) where C_{α} is the C-coefficient in Eq.(F.13) for $|\Xi(x)\rangle$ of Eq.(F.9) with $|\chi(x)\rangle$ equal to $|\psi_{\alpha}(x)\rangle$ of Eq.(6.15). We should keep in mind that A_{α} and C_{α} are, more precisely, $A_{\alpha}^{\alpha_0 \alpha_0}$ and $C_{\alpha}^{\alpha_0 \alpha_0}$.

The asymptotic behavior of the breakup components of $|\phi\rangle$, therefore, is

$$|\phi_{\alpha_0}\rangle - \sum_{\alpha'_0} |\alpha'_0 \phi_{\alpha'_0} F_{\alpha'_0} \rangle \xrightarrow{x \rightarrow \infty} \sum_{\alpha} \int_0^P c_{\alpha} dp |F_{\alpha} \cdot \hat{h}_{\alpha}^{(+)} \rangle B_{\alpha}^{\alpha_0} \quad (6.18)$$

where

$$B_{\alpha}^{\alpha_0} = - \sum_{\alpha'_0} A_{\alpha'_0}^{\alpha_0 \alpha_0} \quad \text{for } \alpha = \alpha(^1S_0) \quad (6.19a)$$

$$= \sum_{\alpha'_0} C_{\alpha'_0}^{\alpha_0 \alpha_0} \quad \text{for all other states} \quad (6.19b)$$

Going back to the Faddeev component $|\phi(1,23)\rangle$ of Eq.(3.1), we have

$$|\psi(1,23)\rangle \xrightarrow[\bar{y} \rightarrow \infty]{x \rightarrow \infty} \sum_{\alpha} \int_0^P c_{\alpha} dp |F_{\alpha}(1) \hat{h}_{\alpha}^{(+)}(23)\rangle \sum_{\alpha_0} \beta_{\alpha_0} B_{\alpha}^{\alpha_0} \quad (6.20)$$

This is for $|\phi_1\rangle$ in Eq.(2.6). Therefore, for the total wave function

$$|\psi\rangle \xrightarrow[\bar{y} \rightarrow \infty]{x \rightarrow \infty} \frac{1}{\sqrt{3}} \sum_{\alpha} \int_0^P c_{\alpha} dp |F_{\alpha}(1) \hat{h}_{\alpha}^{(1)}(23) + F_{\alpha}(2) \hat{h}_{\alpha}(31) + F_{\alpha}(3) \hat{h}_{\alpha}(12)\rangle \sum_{\alpha_0} \beta_{\alpha_0} B_{\alpha}^{\alpha_0} \quad (6.21)$$

The p integral can be carried out using the saddle point method¹³⁾. The result is

$$|\Psi\rangle \xrightarrow[x \rightarrow \infty]{y \rightarrow \infty} \frac{e^{ikr}}{r^{5/2}} \sum_{\alpha} |\alpha(1,23) + \alpha(2,31) + \alpha(3,12)\rangle T_{\alpha}(p_A) \quad , \quad (6.22)$$

$$T_{\alpha}(p_A) = - \frac{1}{\sqrt{3}} \left(\frac{2}{3}\right)^{3/2} i^{1/2} \cdot i^{-(L+l)} k^{3/2} \cdot q_{AP_A}^{L1} \sum_{\alpha_0} \beta_0 B_{\alpha}^{\alpha_0}(p_A) \quad . \quad (6.23)$$

$B_{\alpha}^{\alpha_0}(p_A)$ is given by Eq.(6.19) with p replaced by p_A . Here,

$$p_A = \frac{2k}{3r} y \quad (6.24)$$

$$k = \sqrt{2ME/\hbar^2} \quad (6.25)$$

$$q_A x + p_A y = kr \quad . \quad (6.26)$$

and r is the hyper-radius defined by

$$r = \sqrt{\frac{x^2}{2} + \frac{2}{3}y^2} \quad (6.27)$$

§7. Concluding Remarks

We hope that the presentation in this article of our theory of three-body scattering has been transparent enough to readers who otherwise are not too conversant with the Faddeev theory. We believe that we have made it amply clear that the use of realistic local potentials in the Faddeev theory is as practical as and is not much more complicated than the use of conventional separable approximations. Just as the optical model and DWBA analyses, which were in the realm of theoreticians when we were students(that was in fact a long time ago), are now handled almost routinely by experimentalists, the day will come in the future when nuclear reactions are analysed routinely by using computer codes based on theories such as ours. By then, the justification of conventional(or traditional) nuclear reaction theories will have to be investigated in view of the more mathematically rigorous Faddeev theory. Since the use of complex potentials are not at all prohibited in our theory, we believe the theory presented here will contribute a great deal toward such goals.

Appendix A Partially Separable t-Matrix(PST)

i) Positive energies

An important ingredient in our theory is the method of PST^{11,13,14}). In this appendix, we present a generalized version of it which will be called the source function PST. This appendix also serves as an errata to our previous

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treatments^{11,13,14)} and to show the correct PST for coupled states.

The gist of the PST is as follows¹¹⁾. The Jost function method is useful in treating two-body problems. The expansion in powers of the potential converges absolutely without regards to the strength of the potential. The zeros of the Jost function is the poles of the scattering amplitude. However, in order to carry the method into three-body problems, and to treat the non-pole(non-separable) term of the t matrix as the perturbation, it is necessary to modify the irregular nature of the Jost function. Thus we introduce a function $|\hat{\phi}(x)\rangle$ that is regular and has the same asymptotic behavior as the spherical Hankel function $|h_L^{(+)}(qx)\rangle$. (For $h_L^{(+)}(qx)$, see Eq.(2.18)).

$$|\hat{\phi}(x)\rangle = -G_0 |s(x)\rangle \xrightarrow{x > R_S} |h_L^{(+)}(qx)\rangle \quad . \quad (A.1)$$

Here, $|s(x)\rangle$ is an appropriate short-ranged, regular source function with the normalization

$$\langle \hat{j}_L(qx) | s(x) \rangle = 1 \quad , \quad (A.2)$$

and R_S is its range(See Eq.(2.17) for $\hat{j}_L(qx)$). It is convenient to choose R_S not greater than the range R of the potential V and we shall do so. The free Green function G_0 is decomposed into two terms,

$$G_0 = -|\hat{\phi}\rangle \langle \hat{j} | + \hat{g} \quad , \quad (A.3)$$

which defines \hat{g} . We also introduce the wave operator, \hat{g} as its Green function.

$$\hat{\omega} = 1 + \hat{g} V \hat{\omega} \quad . \quad (A.4)$$

Since $|\hat{\phi}\rangle$ is regular, so are \hat{g} and $\hat{\omega}$. They are real for real and pure imaginary q . Outside the force range

$$\hat{g}V \xrightarrow{x > R} 0 \quad , \quad \hat{\omega} \xrightarrow{x > R} 1 \quad . \quad (A.5)$$

Then the source function PST of $G_0 t$ is given by

$$G_0 t = (\hat{\omega}-1) - \hat{\omega} |\hat{\phi}\rangle \hat{D}^{-1} \langle \hat{j} | V \hat{\omega} \quad (A.6)$$

where

$$\hat{D} = 1 + \langle \hat{j} | V \hat{\omega} | \hat{\phi} \rangle \quad . \quad (A.7)$$

It can be proved that all poles in V are given by the zeros of $\det \hat{D}$, (\hat{D} is a 2×2 matrix for coupled states) and the second term (the separable term) of Eq.(A.6) has the correct pole residues at these poles^{11,16)}. With the properties (A.1) and (A.5), both terms in Eq.(A.6) are regular, and furthermore Eq.(A.6) has all the virtue of the Jost function method provided the operator $\hat{\omega}$ has no poles on or near the integration path (i.e., the positive real q axis below $\sqrt{ME/\hbar^2}$, and the entire positive imaginary q axis). This last condition on $\hat{\omega}$ must be satisfied by a proper choice of the source function $|s(x)\rangle$. One example of such a choice is the use of the Sturm-Liouville functions for uncoupled states. They are defined as the solutions to

$$PG_0 V |\hat{\psi}_n\rangle = \lambda_n |\hat{\psi}_n\rangle \quad (n=1,2,\dots) \quad (\text{A.8})$$

with the normalization

$$\langle \hat{j} | V | \hat{\psi}_n \rangle = -\lambda_n \quad , \quad (\text{A.9})$$

which also yields the asymptotic behavior

$$|\hat{\psi}_n\rangle \xrightarrow{x \rightarrow R} -|\hat{n}(qx)\rangle \quad . \quad (\text{A.10})$$

For $|\hat{n}(qx)\rangle$, see Eq.(2.19). Let us choose the source function $|s(x)\rangle$ as

$$|s(x)\rangle = - \sum_{n=1}^N \alpha_n^{(N)} \frac{V}{\lambda_n} |\hat{\psi}_n\rangle \quad , \quad (\text{A.11})$$

where the summation runs over all eigenstates whose λ_n become larger or close to 1 in the energy interval of interest. The coefficients $\alpha_n^{(N)}$ are those of Eqs.(27) , (28) and (46) of ref. 11. Then, Eq.(A.2) is satisfied by Eq.(A.9) and the normalization condition on $\alpha_n^{(N)}$, Eq.(4.6) of ref. 11.

From Eq.(A.1) we find

$$|\hat{\phi}\rangle = |\hat{\psi} + iq^{L+1} j \rangle \xrightarrow{x > R} |\hat{h}^{(+)}\rangle \quad (\text{A.12})$$

where

$$|\hat{\psi}\rangle = \sum_{n=1}^N \alpha_n^{(N)} |\hat{\psi}_n\rangle \quad . \quad (\text{A.13})$$

In deriving Eq.(A.12), we have used Eq.(A.8) with $G_0 = PG_0 - iq|j\rangle\langle j|$. Therefore, $|\hat{\phi}\rangle$ is regular and has the correct asymptotic form. Incidentally, \hat{D} of

Eq. (A.7) can be expressed as

$$\begin{aligned}\hat{D} &= 1 + \langle j | \hat{V} \omega | \hat{\psi} \rangle + iq \langle j | \hat{V} \omega | j \rangle \\ &= \sum_{n=1}^N (1 - \lambda_n) + iq \langle j | \hat{V} \omega | j \rangle, \end{aligned} \quad (\text{A.14})$$

where we have used Eq. (33) of ref.11. This permits us to rewrite Eq. (A.6) in the many-level form of Eq. (32) of ref.11. What is important, however, is that we have proved in ref.11 that there is no pole in $\hat{\omega}$ in this case. The extension of this method to the optical potential is easily done¹⁵⁾.

A straightforward extension of the above PST for coupled states with the Sturm-Liouville functions proves to have an undesirable aspect. Now, $|\hat{\psi}_n\rangle$ of Eq. (A.8) has two components

$$|\hat{\psi}_n\rangle = \begin{pmatrix} \hat{\psi}_{n,L} \\ \hat{\psi}_{n,L'} \end{pmatrix}.$$

For simplicity, let us consider the case when only λ_1 is chosen to 1 (as in the case of the ${}^3S_1 + {}^3D_1$ two-nucleon state), and henceforth neglect the suffix n . Then, \hat{g} of Eq. (A-3) becomes

$$\hat{g} = PG_0 + |\hat{\psi}\rangle\langle\hat{j}|,$$

where $\langle\hat{j}| = (\langle\hat{j}_L|, \langle\hat{j}_{L'}|)$ while PG_0 is diagonal. This \hat{g} has non-diagonal elements which do not vanish at $x \rightarrow \infty$. As it is indispensable to have Eq. (A.5) for three-body problems, we must modify $|\hat{\psi}\rangle$ so that \hat{g} becomes diagonal. Let us consider

$$|\hat{\chi}\rangle = \begin{pmatrix} |\hat{\psi}_L\rangle & , & 0 \\ 0 & , & |\hat{\psi}_{L'}\rangle \end{pmatrix}$$

together with

$$\langle\hat{j}| = \begin{pmatrix} \langle\hat{j}_L| & , & 0 \\ 0 & , & \langle\hat{j}_{L'}| \end{pmatrix} \quad (\text{A.15})$$

so that

$$\hat{g} = PG_0 + |\hat{\chi}\rangle\langle\hat{j}|$$

is diagonal. Does $\hat{g}V$ approaches to 0 as $x \rightarrow \infty$ as required by Eq. (A.5) ? The asymptotic form of $|\hat{\chi}\rangle$ is given by

$$|\hat{\chi}\rangle \xrightarrow{x \rightarrow R} \begin{pmatrix} |\hat{n}_L\rangle \langle \hat{j}_L | V_{LL} \hat{\psi}_L + V_{LL'} \hat{\psi}_{L'} \rangle / \lambda, & 0 \\ 0 & |\hat{n}_{L'}\rangle \langle \hat{j}_{L'} | V_{L'L} \hat{\psi}_L + V_{L'L'} \hat{\psi}_{L'} \rangle / \lambda. \end{pmatrix}$$

To be $\hat{g}V \xrightarrow{x \rightarrow R} 0$ for this \hat{g} , we must require two conditions

$$\langle \hat{j}_L | V_{LL} \hat{\psi}_L + V_{LL'} \hat{\psi}_{L'} \rangle = -\lambda \quad (\text{A.16})$$

and

$$\langle \hat{j}_{L'} | V_{L'L} \hat{\psi}_L + V_{L'L'} \hat{\psi}_{L'} \rangle = -\lambda$$

be satisfied at the same time. However, $|\hat{\psi}_L\rangle$ and $|\hat{\psi}_{L'}\rangle$ are two components of the solution $|\hat{\psi}\rangle$ of Eq. (A.8) (with $n = 1$), and hence we can have only one freedom about all over normalization. It is not possible to satisfy above two conditions simultaneously.

Thus, we should modify $|\hat{\chi}\rangle$. Let us consider

$$|\hat{\psi}\rangle = \begin{pmatrix} |\hat{\psi}_L\rangle, & 0 \\ 0 & \epsilon |\hat{\psi}_{L'}\rangle \end{pmatrix} \quad (\text{A.17})$$

with the normalization condition Eq. (A.16) and

$$\epsilon = -\lambda / \langle \hat{j}_{L'} | V_{L'L} \hat{\psi}_L + V_{L'L'} \hat{\psi}_{L'} \rangle. \quad (\text{A.18})$$

It is easily seen that this $|\hat{\psi}\rangle$ satisfies Eq. (A.10) with a diagonal $|\hat{n}(qx)\rangle$, and hence

$$\hat{g} = PG_0 + |\hat{\psi}\rangle \langle \hat{j} | \quad (\text{A.19})$$

is not only diagonal but also satisfies $\hat{g}V \xrightarrow{x \rightarrow R} 0$. In the language of the source function PST, if we choose

$$|s(x)\rangle = \begin{pmatrix} |s_L(x)\rangle, & 0 \\ 0 & |s_{L'}(x)\rangle \end{pmatrix} \\ = \begin{pmatrix} -\{V_{LL} |\hat{\psi}_L\rangle + V_{LL'} |\hat{\psi}_{L'}\rangle\} / \lambda, & 0 \\ 0 & -\epsilon \{V_{L'L} |\hat{\psi}_L\rangle + V_{L'L'} |\hat{\psi}_{L'}\rangle\} / \lambda \end{pmatrix} \quad (\text{A.20})$$

as the source function, relations (A.1), (A.2) and (A.12) hold. Then, by the general theory, we have the PST expression of $G_0 t$ as given by Eq. (A.6). We must be careful, however, not to confuse $|\hat{\psi}\rangle$ of Eq. (A.17) with the solu-

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tion $|\hat{\psi}\rangle$ of Eq.(A.8). In fact, $|\hat{\psi}\rangle$ does not satisfy Eq.(A.8) and hence it is not the Sturm-Liouville function. Therefore, the proof in ref.11 concerning the absence of poles in $\hat{\omega}$ does not hold for coupled states.

The question of poles in $\hat{\omega}$ has to be studied case by case, just as for more general choice of the source function $|s(x)\rangle$. Fortunately, in our treatment of the n-d scattering, the unperturbed part I in Eq.(5.11) consists only of the 1S_0 state, which is not coupled. Even the $^3S_1 + ^3D_1$ state can be treated as the perturbation since the deuteron pole is extracted from Γ . This means that the PST expression of $G_0 t$ for positive energy, Eq.(A.6), is required only for the 1S_0 state. Thus, the positive energy contribution to the unperturbed part of Eq.(5.11) is given by

$$\sum_{\alpha} \int_0^{\infty} p_c dp |F_{\alpha}^{\omega} \rangle \langle \tau_{\alpha} F_{\alpha} | = - \sum_{\alpha} \int_0^{\infty} p_c dp |F_{\alpha}^{\omega} \rangle \frac{1}{\hat{D}_a} \langle j_a | V_a^{\omega} | F_{\alpha} | \quad (A.21)$$

with the summation running only over $|\alpha\rangle$ with the 1S_0 two-body state. (See, Table 1). The function \hat{D}_a is given by Eq.(A.14) with $N = 1$. The contribution from $(\hat{\omega} - 1)$ is included in the perturbation W_{α} .

ii) Negative energies

The general theory of source function PST presented in (i) can in principle be applied to negative energies as well. Strictly speaking, the PST for coupled states must be treated with the same care as for the positive energies. However, since G_0 approaches $e^{-|q|x}$ asymptotically for negative energies, even coupled states can be treated by the Sturm-Liouville functions in the same way as uncoupled states. In fact, this is the method we have employed in calculating the triton and ^3He bound state problems^{3,4,17}). Now, the Sturm-Liouville function $|\hat{\psi}\rangle$ with the largest eigenvalue λ is defined by

$$G_0 V |\hat{\psi}\rangle = \lambda |\hat{\psi}\rangle \quad (A.22)$$

with the normalization

$$\langle \hat{\psi} | V | \hat{\psi} \rangle = -1 . \quad (A.23)$$

We introduce g and the corresponding wave operator ω by

$$G_0 = -\lambda |\hat{\psi}\rangle \langle \hat{\psi}| + g \quad (A.24)$$

$$\omega = 1 + g V \omega . \quad (A.25)$$

Here, g and ω are both regular at the origin and real. For $x > R$, g becomes

proportional to $h_L^{(+)}(iqx)$. Then we can show that¹³⁾

$$G_o t = (\omega - 1) - |\hat{\psi}\rangle \frac{\lambda}{1 - \lambda} \langle \hat{\psi} | V \quad (A.26)$$

The negative energy contribution to the unperturbed part I of Eq.(5.11) consists of the 1S_o state with $|q| < \bar{q}$ (or $p_c < p < \bar{p}$). Thus, in Eq.(5.11),

$$\sum_{\alpha} \int_{p_c}^{\bar{p}} dp |F_{\alpha} \nu \rangle \langle \tau_{\alpha} F_{\alpha} | = - \sum_{\alpha} \int_{p_c}^{\bar{p}} dp |F_{\alpha} \tilde{\psi}_{\alpha} \rangle \frac{\lambda}{1 - \lambda} \langle \tilde{\psi}_{\alpha} | V(F_{\alpha} | \quad (A.27)$$

See, Table 1. The contribution from $(\omega - 1)$ is included in W_{α} .

Appendix B Treatment of perturbation near the deuteron pole

Theoretically there is no deuteron pole in Γ of Eq.(3.5). The contribution to Γ from the $^3S_1 + ^3D_1$ two-body state is given by

$$\Gamma^D = \sum_{\alpha_o} \int_0^{\infty} dp |F_{\alpha_o} \rangle [G_{\alpha_o} V - |\phi_d \rangle \frac{1}{q^2 + q_d^2} \langle \phi_d | V] (F_{\alpha_o} | \quad (B.1)$$

The cancellation of the deuteron pole of GV and $|\phi_d \rangle \frac{1}{q^2 + q_d^2} \langle \phi_d | V$ is tricky for numerical treatment. When q is not too close to the deuteron pole iq_d , we may use Eq.(B.1) directly. When $|q|$ is close to q_d , we employ the PST expression of $G_o t$ of Eq.(A.26) and rewrite inside the square bracket of Eq.(B.1) as

$$GV - |\phi_d \rangle \frac{1}{q^2 + q_d^2} \langle \phi_d | V = (\omega - 1) - P(|q|) V \quad (B.2)$$

where

$$P(|q|) = |\tilde{\psi}\rangle \frac{\lambda}{1 - \lambda} \langle \tilde{\psi} | + |\phi_d \rangle \frac{1}{-|q|^2 + q_d^2} \langle \phi_d | \quad (B.3)$$

with

$$|\hat{\psi}\rangle = \begin{pmatrix} |\tilde{\psi}(^3S_1)\rangle \\ |\tilde{\psi}(^3D_1)\rangle \end{pmatrix} \quad (B.4)$$

This is given by the solution of Eq.(A.22) with the normalization (A.23). Since we can show that

$$\frac{d\lambda(q)}{d|q|} = -2|q|\lambda^2 \langle \tilde{\psi} | \tilde{\psi} \rangle \quad (B.5)$$

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the deuteron poles in the first term and the second term of $P(|q|)$ cancel each other. Thus $P(q_d)$ is finite. In fact, we have

$$P(q_d) = |\overset{0}{\psi}_o\rangle\langle\psi_p^{(1)}| + |\phi_d\rangle\langle\psi_p^{(2)}|, \quad (\text{B.6})$$

where

$$\langle\psi_p^{(1)}| = -\frac{1}{\sigma} \frac{1}{\lambda_o} \langle\overset{0}{\psi}_o| \quad (\text{B.7})$$

and

$$\langle\psi_p^{(2)}| = -\frac{N_o}{\sigma} \frac{1}{\lambda_o} \langle\overset{0}{\psi}_o| + \left\{ \frac{1}{2q_d} \left(\overset{0}{\lambda}_o - \frac{\overset{0}{\lambda}}{2\lambda_o} \right) + \frac{1}{4q_d^2} \right\} \langle\phi_d| \quad (\text{B.8})$$

where $N_o = (\langle\overset{0}{\psi}_o|\overset{0}{\psi}_o\rangle)^{1/2}$, $\overset{0}{\lambda}$ indicates d/dq , and the suffix o is to evaluate the quantity at $|q| = q_d$. The value of p that corresponds to q_d is p_o of Eq. (2.3). If the integration mesh point p is very close to p_o , we evaluate the integrand of Eq. (B.1) by interpolation using the value at p_o (to which we use Eqs. (B.3) and (B.6)) and the value at neighboring mesh points (to which we use Eq. (B.1) directly). This will necessitate a special treatment for the contribution from the asymptotic region of $P(|q|)$ as explained in Appendix C.

Appendix C Reduction of $(F_{\alpha} | Q | F_{\alpha}, Z_{\alpha}, \rangle$

The calculation of $(F_{\alpha} | Q | F_{\alpha}, Z_{\alpha}, \rangle$ is the center of the entire operation. The algebra involved can be dealt with by the method of ref. 18. Throughout this appendix, we use the notation of Eqs. (2.17), (2.18) and (2.19).

First, we consider the case when $|Z_{\alpha}, (q'x)\rangle$ has the following asymptotic form,

$$|Z_{\alpha}, (q'x)\rangle \xrightarrow{x>R} A_{\alpha}, (q') |h_{L'}^{(+)}(q'x)\rangle. \quad (\text{C.1})$$

The exceptional cases are the terms $-|\phi_d\rangle \frac{1}{q^2 + q_d^2} \langle\phi_d|v$ and $-P(|q|)v$ in w_{α} for the ${}^3S_1 + {}^3D_1$ state. These will be treated later in this appendix. Using Eqs. (E.24) and (E.25) of ref. 18 for $|Z_{\alpha}\rangle$ with the asymptotic form (C.1), we find

$$(F_{\alpha} | Q | F_{\alpha}, Z_{\alpha}, \rangle = \sum_{L_o S_o \gamma} C_{\alpha\alpha'}^{\gamma}(p, p') [X_{L_o}^{\gamma}(p, p'; x) + A_{\alpha}, (q') Y_{L'}^{\gamma}(p, p'; x)], \quad (\text{C.2})$$

where

$$C_{\alpha\alpha'}^{\gamma}(p, p') = \frac{2}{\pi} N_{\alpha\alpha'}^{(L_o S_o)} S_{(L_o, L', \ell')}^{\gamma}(p, p') \quad (\text{C.3})$$

with $N_{\alpha\alpha'}^{(L_0 S_0)}$ and $S_{(L\ell, L'\ell')}^{\gamma}_{L_0}(p, p')$ given by Eqs. (E.7) and (E.25) of ref.18.

$$N_{\alpha\alpha'}^{(L_0 S_0)} = \delta_{L_0 L'_0} \delta_{S_0 S'_0} \hat{J} \hat{j} \hat{L}_0 \hat{S}_0 \begin{Bmatrix} L & \ell & L_0 \\ S & \frac{1}{2} & S_0 \\ J & j & J_0 \end{Bmatrix} \hat{J}' \hat{j}' \hat{L}'_0 \hat{S}'_0 \begin{Bmatrix} L' & \ell' & L'_0 \\ S' & \frac{1}{2} & S'_0 \\ J' & j' & J'_0 \end{Bmatrix} \\ \times (-)^{I \hat{I} \hat{I}'} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & I \\ \frac{1}{2} & T & I' \end{Bmatrix} (-)^{S \hat{S} \hat{S}'} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S \\ \frac{1}{2} & S_0 & S' \end{Bmatrix}, \quad (C.4)$$

$$S_{(L\ell, L'\ell')}^{\gamma}_{L_0}(p, p') = \sum_{a=0}^L \sum_{a'=0}^{L'} p^{a+a'+1} p'^{b+b'+1} R_{(L\ell, L'\ell')}^{aa'\gamma}_{L_0}, \quad (b=L-a) (b'=L'-a') \quad (C.5)$$

where

$$R_{(L\ell, L'\ell')}^{aa'\gamma}_{L_0} = \hat{\ell} \hat{\ell}' \hat{L} \hat{L}' \hat{b} \hat{b}' \hat{\gamma} \begin{pmatrix} 2L+1 \\ 2a \end{pmatrix}^{1/2} \begin{pmatrix} 2L'+1 \\ 2a' \end{pmatrix}^{1/2} \left(-\frac{1}{2}\right)^a (-1)^b (1)^{a'} \left(\frac{1}{2}\right)^{b'} \\ \times i^{\ell-\ell'+L-L'} (-)^{L+\ell+L_0+a} \sum_c (-)^c \langle c | a_0 a' | c \rangle \langle \ell 0 c | \gamma 0 \rangle \\ \times \sum_g \langle b_0 \gamma 0 | g 0 \rangle \langle \ell' 0 b' | g 0 \rangle \begin{Bmatrix} g & b' & \ell' \\ L' & L_0 & a' \end{Bmatrix} \begin{Bmatrix} L & \ell & L_0 \\ a & c & a' \\ b & \gamma & g \end{Bmatrix}. \quad (C.6)$$

The function $X_{L\alpha}^{\gamma}(p, p'; x)$ in Eq. (C.2) is defined by

$$X_{L\alpha}^{\gamma}(p, p'; x) = \int_{-1}^1 du P_{\gamma}(u) \hat{j}_L(\lambda x) [\rho_{\alpha'}^{(A)}(\lambda', q') + A_{\alpha'}(q') \rho_{\alpha'}^{(B)}(\lambda', q')] \quad (C.7)$$

where

$$\rho_{\alpha'}^{(A)}(\lambda', q') = \int_0^R x'^2 dx' \hat{j}_{L'}(\lambda' x') z_{\alpha'}(q' x') \quad (C.8)$$

and

$$\rho_{\alpha'}^{(B)}(\lambda', q') = - \int_0^R x'^2 dx' \hat{j}_{L'}(\lambda' x') \hat{h}_{L'}^{(+)}(q' x') \quad (C.9)$$

Here

$$\vec{\lambda} = -\frac{\vec{p}}{2} - \vec{p}' \quad \text{and} \quad \vec{\lambda}' = \vec{p} + \frac{\vec{p}'}{2} \quad (C.10)$$

are the relative momenta of the interacting pairs (1,2) and (2,3), respec-

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tively, off the three-body energy shell. The function $\rho_{\alpha'}^{(B)}(\lambda'; q')$ can be given analytically. For λ' not too close to q' , we have

$$\rho_{\alpha'}^{(B)}(\lambda'; q') = - \frac{1}{\lambda'^2 - q'^2} \{ R^2 q'^2 \hat{j}_{L'}(\lambda'R) \hat{h}_{L'-1}^{(+)}(q'R) - R^2 \hat{j}_{L'-1}(\lambda'R) \hat{h}_{L'}^{(+)}(q'R) + 1 \} \quad (C.11)$$

For $\lambda' \approx q'$, we better use

$$\rho_{\alpha'}^{(B)}(\lambda'; q') = - \frac{R^2}{\lambda' + q'} \left\{ q'^2 \frac{\hat{j}_{L'}(\lambda'R) - \hat{j}_{L'}(q'R)}{\lambda' - q'} \hat{h}_{L'-1}^{(+)}(q'R) - \frac{\hat{j}_{L'-1}(\lambda'R) - \hat{j}_{L'-1}(q'R)}{\lambda' - q'} \hat{h}_{L'}^{(+)}(q'R) \right\} \quad (C.12)$$

For $\lambda' = q'$, we have

$$\rho_{\alpha'}^{(B)}(q', q') = - \frac{R^2}{2} \{ (-(2L+1) \hat{j}_{L'}(q'R) + R \hat{j}_{L'-1}(q'R)) \hat{h}_{L'-1}^{(+)}(q'R) + R \hat{j}_{L'}(q'R) \hat{h}_{L'}^{(+)}(q'R) \} \quad (C.13)$$

In the above expressions, we need the following functions for $L = 0$,

$$\hat{j}_{-1}(\lambda x) = -\lambda n_0(x), \quad \hat{h}_{-1}^{(+)}(qx) = \frac{i}{q} \hat{h}_0^{(+)}(qx) \quad (C.14)$$

Both $\rho_{\alpha'}^{(A)}(\lambda', q')$ and $\rho_{\alpha'}^{(B)}(\lambda', q')$ have no singularities. The function $Y_L^Y(p, p'; x)$ in Eq. (C.2) is defined by

$$Y_L^Y(p, p'; x) = \int_{-1}^1 du P_Y(u) \hat{j}_L(\lambda x) \int_0^\infty x'^2 dx' \hat{j}_{L'}(\lambda' x') \hat{h}_{L'}^{(+)}(q' x') \quad (C.15)$$

If we use the formula given by Fuda¹⁹⁾,

$$\begin{aligned} \int_0^\infty x'^2 dx' \hat{j}_{L'}(\lambda' x') \hat{h}_{L'}^{(+)}(q' x') &= \frac{1}{\lambda'^2 - (q'^2 + i\epsilon)} \\ &= \frac{1}{ME/\hbar^2 - p^2 - p'^2 - pp'u + i\epsilon} \end{aligned} \quad (C.16)$$

which may be identified as (-1) times the free three-body Green function $G_0 =$

$(\hbar^2/M)/(E - H_0 + i\varepsilon)$, we find

$$Y_L^\gamma(p, p'; x) = - \int_{-1}^1 du P_\gamma(u) \frac{\hat{j}_L(\lambda x)}{ME/\hbar^2 - p^2 p'^2 - pp'u + i\varepsilon} \quad (C.17)$$

$$= - \frac{1}{pp'} \int_{-1}^1 du P_\gamma(u) \frac{\hat{j}_L(\lambda x)}{(u_0(p, p') + i\varepsilon) - u} \quad (C.18)$$

Here we have defined

$$u_0(p, p') = \frac{ME/\hbar^2 - p^2 - p'^2}{pp'} \quad (C.19)$$

We decompose Y_L^γ into two terms

$$Y_L^\gamma(p, p'; x) = - \frac{1}{pp'} \left[\int_{-1}^1 du P_\gamma(u) \frac{\hat{j}_L(\lambda x) - \hat{j}_L(\lambda_0 x)}{u_0 - u} \right. \quad (C.20)$$

$$\left. + 2\hat{j}_L(\lambda_0 x) Q_\gamma(u_0 + i\varepsilon) \right]. \quad (C.21)$$

Here we have defined λ_0 by

$$\lambda_0 = \lambda(u = u_0) = \alpha \quad \text{for } 0 < p < p_c, \quad (C.22a)$$

$$= \lambda(u = -1) = \left| \frac{p}{2} - p' \right| \quad \text{for } p > p_c. \quad (C.22b)$$

The second Legendre function $Q_\gamma(z)$ is defined by²⁰⁾

$$Q_\gamma(z) = \frac{1}{2} \int_{-1}^1 \frac{P_\gamma(u)}{z - u} du \quad (C.23)$$

$$= \frac{1}{2} P_\gamma(z) \ln \frac{z+1}{z-1} - W_{\gamma-1}(z), \quad (C.24)$$

where

$$W_{\gamma-1}(z) = \sum_{k=0}^{\gamma-1} \frac{(2k+1)[1 - (-1)^{\gamma+k}]}{(\gamma-k)(\gamma+k+1)} P_k(z) \quad (\gamma \geq 1), \quad (C.25)$$

and

$$W_{-1}(z) = 0, \quad W_0(z) = 1. \quad (C.26)$$

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The function $Q(z)$ has logarithmic singularities at $z = \pm 1$. Therefore, $Y_L^Y(p, p'; x)$ has logarithmic singularities on the curves defined by $u_0 + i\epsilon = \pm 1$. The roots of these equations are

$$p' = \nu(p, s) \equiv -\frac{p}{2} + s \quad (\text{C.27a})$$

$$p' = \mu(p, s) \equiv \frac{p}{2} + s \quad (\text{C.27b})$$

$$p' = -\nu(p, s) \quad (\text{C.27c})$$

and

$$p' = -\mu(p, s) , \quad (\text{C.27d})$$

where

$$s = \sqrt{b^2 - p^2} \quad , \quad b = \sqrt{p_c^2 + i\epsilon} \quad . \quad (\text{C.28})$$

For real positive p and p' in the limit of $\epsilon \rightarrow 0$, these roots are given by the curves in Fig.13. Since $-1 < u_0 < 1$ within this crescent shaped region, the integrand in Eq.(C.18) has poles at $u = u_0$. Since u runs from -1 to 1 continuously, these poles constitute a cut running from $u_0 = -1$ to 1 . The discontinuity of $Q_Y(u_0)$ across the cut is easily obtained from Eq.(C.23) to be $-i\pi P_Y(u_0)$, which is twice the imaginary part of $Q_Y(u_0 + i\epsilon)$. Therefore, $Y_L^Y(p, p'; x)$ is complex within the crescent shaped region with the imaginary part given by

$$\text{Im } Y_L^Y(p, p'; x) = \frac{\pi}{pp'} \hat{j}_L(\lambda_0 x) P_Y(u_0) \theta(1 - |u_0|). \quad (\text{C.29})$$

Of course, this can be obtained directly from Eq.(C.18).

For $q = i|q|$ (negative two-body energies), p is greater than p_c , and there is neither logarithmic singularities nor imaginary part. Since $q = i|q|$, Eq.(C.22a) is inappropriate because $\hat{j}_L(qx)$ would diverge as $x \rightarrow \infty$. Hence, we switch the definition of λ_0 to Eq.(C.22b). This is to take care of the most dangerous contribution to Eq.(C.20) from $u = -1$ where the denominator $u_0 - u$ takes the least absolute value ($u_0 < -1$ here). For p sufficiently far from p_c , we may use Eq.(C.18) directly instead of Eqs.(C.20) and (C.21).

The terms $-\langle \phi_d | \frac{1}{q^2 + q_d^2} | \phi_d \rangle V$ and $-P(|q|)V$ in $W_{\mathcal{Q}}$ for the ${}^3S_1 + {}^3D_1$

state are exceptions to Eq.(C.1). As explained in Appendix B, $P(|q|)V$ is treated by interpolation using the value at $|q| = q_d$ given by Eq.(B.6). For the second term $-|\phi_d\rangle \frac{1}{q^2 + q_d^2} \langle \phi_d|V$, the asymptotic form of $|z_\alpha(x)\rangle$ takes the form

$$|z_\alpha(x)\rangle \xrightarrow{x > R} A_\alpha(q') \hat{h}_L^{(+)}(iq_d x) \quad (C.30)$$

$\hat{h}_L^{(+)}(i|q|x)$ is a real function of a real variable $|q|x$. Therefore, all the formulas from Eq.(C.2) through Eq.(C.16) can be applicable with iq_d in place of q' . Since $\lambda'^2 - q'^2$ now reads $\lambda'^2 + q_d^2$, which is not only positive definite but also not even close to zero, we may perform the integrations in Eq.(C.15) without worrying about singularities. (There is no need for Eqs.(C.12) and (C.13) either.)

The only true exception, therefore, is the first term $|\psi_0\rangle \langle \psi_p^{(1)}|$ in Eq.(B.6) evaluated at $|q| = q_d$. To treat this term, we shall have to compute and store in advance the integration

$$\tilde{\rho}_L(\lambda') \equiv \int_0^\infty x'^2 dx' \hat{j}_L(\lambda'x') \hat{\psi}_0(q_d x'). \quad (C.31)$$

This has no singularities. Since $|z_\alpha\rangle$ is given either by Eq.(6.8) or Eq.(6.13), the contribution of $|\tilde{\psi}_0\rangle \langle \psi_p^{(1)}|$ in $P(q_d)$ to $(F_\alpha |Q| F_\alpha |z_\alpha\rangle$ takes the form

$$\sum_{L_0 S_0} C_{\alpha\alpha}^Y(p,p') \int_{-1}^1 du P_Y(u) \hat{j}_L(\lambda x) \hat{\rho}_L(\lambda') \langle \psi_p^{(1)}|V|n, \text{ or } \zeta\rangle. \quad (C.32)$$

Appendix D Reduction of $(F_\alpha |Q| \alpha_0 \phi_d \chi\rangle$

For the zeroth order term of M of Eq.(5.16), we must compute $(F_\alpha |Q| \alpha_0 \phi_d \chi\rangle$, where $|\chi\rangle$ is the i -th iteration $|\xi^{(i)}\rangle$ when we are solving Eq.(5.3), or $|\chi\rangle$ is the elastic component $|F\rangle$ when we are computing $|\phi\rangle$ of Eq.(5.2). In either case, $|\chi\rangle$ is a distorted spectator wave function. The formulas to compute $(F_\alpha |Q| \alpha' \phi_d \chi\rangle$ have already been presented in ref.4. There are, however, some errors in the phase of these formulas, which result in an extra phase factor $(-)^{L+L_0+L}$ that should be multiplied to the coefficient $R_{(L\ell, L'\ell')}^{aco} L_0$. Below we summarize these formulas with this correction.

$$(F_\alpha |Q| \alpha' \phi_d \chi\rangle = 2 \sum_{L_0 S_0} N_{\alpha \alpha'}^{(L_0 S_0)} m_{\alpha\alpha'}^{L_0}(x) \quad (\alpha' = \alpha_0) \quad (D.1)$$

with $N_{\alpha\alpha'}^{(L_0 S_0)}$ given by Eq.(C.6), and

$$m_{\alpha\alpha'}^{L_0}(x) = \int_0^\infty y^2 dy u_\ell(p,y) U_{\alpha\alpha'}^{L_0}(x,y) \quad (D.2)$$

For $u_\ell(p,y)$, see Eq.(5.7). $U_{\alpha\alpha'}^{L_0}(x,y)$ is given by

$$U_{\alpha\alpha'}^{L_0}(x,y) = \sum_{a=0}^{L'} \sum_{c=0}^{\ell'} \sum_{\sigma} x^{a+c} y^{b+d} K_{\sigma}^{\alpha'}(x,y) R_{(L\ell, L'\ell')}^{ac\sigma}_{L_0} \quad (D.3)$$

(b=L'-a) (d=\ell'-c)

where

$$R_{(L\ell, L'\ell')}^{ac\sigma}_{L_0} = (-)^{L+L_0} \hat{\ell} \hat{L} \hat{L}' \hat{\ell}' (-)^{\sigma} \hat{\sigma}^{2bd} \binom{2L'+1}{2a}^{1/2} \binom{2\ell'+1}{2c}^{1/2}$$

$$\times (-\frac{1}{2})^a (1)^b (-\frac{3}{4})^c (-\frac{1}{2})^d \sum_{\lambda\beta} \begin{pmatrix} L & \lambda & \sigma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell & \rho & \sigma \\ 0 & 0 & 0 \end{pmatrix} \hat{\rho}^2 \hat{\lambda}^2 \begin{pmatrix} a & c & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} b & d & \rho \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{Bmatrix} \lambda & \sigma & L \\ \ell & L_0 & \rho \end{Bmatrix} \begin{Bmatrix} a & b & L' \\ c & d & \ell' \\ \lambda & \rho & L_0 \end{Bmatrix} \quad (D.4)$$

and

$$K_{\sigma}^{\alpha'}(x,y) = \frac{1}{2} \int_{-1}^1 d(\cos\theta) \frac{X(Y'')}{x^{\ell'} y^{\ell'}} \frac{\phi_d(x'')}{x''^{L'}} P_{\sigma}(\cos\theta_{x'y}) \quad (D.5)$$

Here

$$\vec{x}'' = -\frac{1}{2} \vec{x} + \vec{y} \quad , \quad \vec{y}'' = -\frac{3}{4} \vec{x} - \frac{1}{2} \vec{y} \quad (D.6)$$

Appendix E Iterative solution of Eq.(5.3)

The stationary solution $|\xi\rangle$ of the elastic channel satisfies Eq.(5.3).

$$|\xi\rangle = |j\rangle + PG_0^{\check{}} \langle \phi_d | \bar{V}Q (1 - \Gamma Q)^{-1} | \phi_d \xi \rangle \quad (E.1)$$

Introducing the non-local potential U by Eq.(3.14)

$$U = \langle \phi_d | \bar{V}Q (1 - \Gamma Q)^{-1} | \phi_d \rangle \quad , \quad (E.2)$$

we express Eq.(E.1) in a compact form of Eq.(4.5).

$$|\xi\rangle = |j\rangle + PG_0^{\check{}} U |\xi\rangle \quad (E.3)$$

In this form, we can employ the iterative scheme of ref.7. Starting with

$$|f^{(0)}\rangle = |j\rangle, \quad |\xi^{(0)}\rangle = |\xi\rangle \text{ and } U^{(0)} = U \quad (\text{E.4})$$

we construct successively for $i = 0, 1, 2, \dots$

$$U^{(i+1)} = U^{(i)} - \frac{U^{(i)} |f^{(i)}\rangle \langle f^{(i)}| U^{(i)}}{\langle f^{(i)} | U^{(i)} | f^{(i)} \rangle} \quad (\text{E.5})$$

$$|f^{(i+1)}\rangle = P_{G_0} U^{(i)} |f^{(i)}\rangle. \quad (\text{E.6})$$

$U^{(i+1)}$ is orthogonal to all $|f^{(j)}\rangle$, $0 \leq j \leq i$. We can reason that⁷⁾ at a certain stage we may set with good accuracy

$$|\xi^{(N)}\rangle = |f^{(N)}\rangle. \quad (\text{E.7})$$

Then, by going backwards using

$$|\xi^{(i)}\rangle = |f^{(i)}\rangle + |\xi^{(i+1)}\rangle \frac{\langle f^{(i)} | U^{(i)} | f^{(i)} \rangle}{\langle f^{(i)} | U^{(i)} | f^{(i)} \rangle - \langle f^{(i)} | U^{(i)} | \xi^{(i+1)} \rangle} \quad (\text{E.8})$$

we find

$$|\xi\rangle = |\xi^{(0)}\rangle.$$

This method has been tested in a variety of cases, not only for non-local potentials but also for local potentials. Despite the fact that this is an iterative scheme, it works beautifully even for potentials deep enough to have a number of bound states. This method amounts to replacing the original potential U by a sum of a finite number of separable terms. Nevertheless, it works for local potentials as well. This opens up a very interesting possibility of effectively approximating a local potential by a finite number of separable terms, in spite of the argument against it²¹⁾.

The method of continued fraction (MCF) for the scattering matrix⁷⁾ is a sophisticated version of the above method. The MCF works very efficiently for the case when the potential is simple enough to allow storage in the computer memory. Our non-local potential U , however, is extremely complicated with the operator $(1 - \Gamma Q)^{-1}$ in it, the operation of which essentially amounts to solving the three-body problem itself. Therefore, it is out of

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question to store U itself. Instead, we go back to the original method. This requires the storage of $|f^{(i)}\rangle$ and $U^{(i)}|f^{(i)}\rangle$ at each iteration. This is much easier in practice. Thus, we proceed as follows.

We need semi-permanent storage places for $|f^{(i)}\rangle$, $U^{(i)}|f^{(i)}\rangle$ and $U_{ki} \equiv \langle f^{(k)}|U^{(k)}|f^{(i)}\rangle$ for $i \leq N$, $k \leq i$, quantities which are needed until the end of the process of iteration. We also need a temporary memory space for $U^{(i)}|f^{(i+1)}\rangle$, the space which can be used repeatedly for all iterations.

To begin, we compute and store

$$|f^{(0)}\rangle, \quad U^{(0)}|f^{(0)}\rangle \text{ and } U_{00} \quad (\text{E.9})$$

from which we calculate

$$|f^{(1)}\rangle = PG_0 U^{(0)}|f^{(0)}\rangle, \quad U^{(0)}|f^{(1)}\rangle, \text{ and } U_{01}. \quad (\text{E.10})$$

Then, we repeat the following computations from Eq.(E.11) to Eq.(E.17) for $1 \leq i \leq N-1$.

$$U^{(i)}|f^{(i)}\rangle = U^{(i-1)}|f^{(i)}\rangle - U^{(i-1)}|f^{(i-1)}\rangle \frac{U_{i-1,i}}{U_{i-1,i-1}} \quad (\text{E.11})$$

$$U_{ii} \quad (\text{E.12})$$

$$|f^{(i+1)}\rangle = PG_0 U^{(i)}|f^{(i)}\rangle \quad (\text{E.13})$$

$$U^{(0)}|f^{(i+1)}\rangle \quad (\text{E.14})$$

$$U_{0,i+1} \quad (\text{E.15})$$

For $1 \leq j \leq i$, we compute

$$U^{(j)}|f^{(i+1)}\rangle = U^{(j-1)}|f^{(i+1)}\rangle - U^{(j-1)}|f^{(j-1)}\rangle \frac{U_{j-1,i+1}}{U_{j-1,j-1}} \quad (\text{E.16})$$

$$U_{j,i+1} \quad (\text{E.17})$$

Having completed the above calculations, we re-set

$$|\xi^{(N)}\rangle = |f^{(N)}\rangle$$

and

$$\langle f^{(j)}|U^{(j)}|\xi^{(N)}\rangle = U_{jN}, \quad \text{for } 0 \leq j \leq N-1. \quad (\text{E.18})$$

For $N - 1 \geq j \geq 1$ downward, we compute from Eq. (E.19) to Eq. (E.21)

$$c_j = \frac{U_{jj}}{U_{jj} - \langle f^{(j)} | U^{(j)} | \xi^{(j+1)} \rangle} \quad (\text{E.19})$$

$$|\xi^{(j)}\rangle = |f^{(j)}\rangle + |\xi^{(j+1)}\rangle c_j \quad (\text{E.20})$$

and for $0 \leq k \leq j - 1$

$$\langle f^{(k)} | U^{(k)} | \xi^{(j)} \rangle = U_{kj} + \langle f^{(k)} | U^{(k)} | \xi^{(j+1)} \rangle c_j . \quad (\text{E.21})$$

Finally, we find

$$|\xi^{(0)}\rangle = |f^{(0)}\rangle + |\xi^{(1)}\rangle \frac{U_{00}}{U_{00} - \langle f^{(0)} | U^{(0)} | \xi^{(1)} \rangle} . \quad (\text{E.22})$$

Of course, we must check the convergence.

During the whole process, the major task is the calculation of $U^{(0)} |f^{(0)}\rangle$ and $U^{(0)} |f^{(i+1)}\rangle$ in Eqs. (E.9) and (E.14) which requires the operation of $(1 - \Gamma Q)^{-1}$ as explained in section 5. The rest of the calculation is very minor. The computation of $|f^{(i+1)}\rangle$ of Eq. (E.13) can be done most easily by solving

$$\left[\frac{d^2}{dy^2} + \frac{2}{y} \frac{d}{dy} - \frac{\ell(\ell+1)}{y^2} + p_0^2 \right] |f^{(i+1)}\rangle = U^{(i)} |f^{(i)}\rangle \quad (\text{E.23})$$

with the boundary condition that $|f^{(i+1)}\rangle$ be regular at the origin and

$$|f^{(i+1)}\rangle \xrightarrow{y > R_U} p_0 |n_\ell(p_0 y)\rangle + j_\ell(p_0 y) |U^{(i)} |f^{(i)}\rangle , \quad (\text{E.24})$$

where R_U is the range of $U^{(i)}$. Let y_M be the matching point of the inner solution ($y < y_M$) and the outer solution ($y > y_M$). Also, let $|f_{in}^P\rangle$ be the regular inner particular solution of Eq. (E.23), and $|f_{out}^P\rangle$ be the outer particular solution inwardly solved from outside starting with $f_{out}^P = f_{out}^{P'} = 0$ at R_U . Then

$$|f^{(i+1)}\rangle = \beta |j_\ell(p_0 y)\rangle + |f_{in}^P\rangle , \text{ for } y < y_M \quad (\text{E.25})$$

and

$$|f^{(i+1)}\rangle = \alpha |n_\ell(p_0 y)\rangle + |f_{out}^P\rangle , \text{ for } y > y_M . \quad (\text{E.26})$$

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By matching the values and the derivatives of inner and outer solutions at $y = y_M$, we obtain α and β . It can easily be shown that α thus obtained is in fact equal to $\langle j_\ell(p_O y) | U^{(i)} | f^{(i)} \rangle$.

Appendix F Operators $(\omega - 1)$, $(\hat{\omega} - 1)$ and GV

As stated in Appendix A, we treat the negative energy PST by the Sturm-Liouville functions. As a result, the treatment of $(\omega - 1)$ and GV for the negative energy states is identical with that of ref.3, and we shall not repeat it here. We wish to comment, though, that if we did not use the Strumian PST but a more general source function PST, the treatment need be modified slightly since then we do not have the relation $\langle \hat{\psi} | V_\omega = \langle \hat{\psi} | V$. This relation applies only to the Strum-Liouville function $|\hat{\psi}\rangle$. We also should point out that the asymptotic form of the interaction pair is better to be made proportional to $\hat{h}_L^{(+)}(i|q|x)$ of Eq.(2.18) rather than $h_L^{(+)}(q|x)$ of ref.3.

As we have stated in section 5 and in Appendix A, the only state that should be treated as the unperturbed part in Γ is the 1S_0 state. Therefore, $(\omega - 1)$ and $(\hat{\omega} - 1)$ are needed only for this state. For the 1S_0 state with positive energies, we have also stated in Appendix A that we can use the Sturm-Liouville function $|\hat{\psi}\rangle$ with the largest eigenvalue λ with the source function $s(x) = -\hat{V}|\hat{\psi}\rangle/\lambda$ of Eq.(A.11).

To compute $(\hat{\omega} - 1)|\chi\rangle$, where $|\chi\rangle$ is a given function of x that is regular, let us define

$$|x(x)\rangle = (\hat{\omega} - 1)|\chi\rangle \quad . \quad (F.1)$$

Using Eqs.(A.3) and (A.4), we find

$$\begin{aligned} |x\rangle &= \hat{g}\hat{\omega}|\chi\rangle = [G_0 + |\hat{\phi}\rangle\langle\hat{j}|] \hat{V}\hat{\omega}|\chi\rangle \\ &= [G_0 + |\hat{\phi}\rangle\langle\hat{j}|] \hat{V}|x + \chi\rangle \quad . \end{aligned} \quad (F.2)$$

The corresponding differential equation is

$$\begin{aligned} \left[\frac{d^2}{dx^2} + \frac{2}{x} \frac{d}{dx} - \frac{L(L+1)}{x^2} + q^2 - V(x) \right] X(x) \\ = -s(x)\langle\hat{j}| \hat{V}|x + \chi\rangle + V(x)\chi(x) \quad . \end{aligned} \quad (F.3)$$

Here $X(x)$ should be regular. It must vanish at $x > R$ (See, Eq.(A.5)).

Let us denote the homogeneous regular solution for $x < x_M$ by $X_{in}^H(x)$, and define the inner and outer particular solutions $X_{in,out}^P$ and $\Pi_{in,out}^P$ by

$$\left[\frac{d^2}{dx^2} + \frac{2}{x} \frac{d}{dx} - \frac{L(L+1)}{x^2} + q^2 - V(x) \right] X^P(x) = -s(x) \quad (F.4)$$

and

$$\left[\frac{d^2}{dx^2} + \frac{2}{x} \frac{d}{dx} - \frac{L(L+1)}{x^2} + q^2 - V(x) \right] \Pi^P(x) = V(x)\chi(x) \quad (F.5)$$

Here, X_{in}^P and Π_{in}^P are both regular and for $x < x_M$, and X_{out}^P and Π_{out}^P are for $x_M < x < R$ which are obtained by solving Eqs.(F.4) and (F.5) inward from outside by starting $X^P = X^{P'} = 0$ and $\Pi^P = \Pi^{P'} = 0$ at $x = R$. Then the inner solution ($x < x_M$) and the outer solution ($x > x_M$) to Eq.(F.3) are given by

$$|X(x)\rangle = |X_{in}^H(x)\rangle c + |X_{in}^P\rangle \alpha + |\Pi_{in}\rangle, \quad \text{for } x < x_M \quad (F.6)$$

$$|X(x)\rangle = |X_{out}^P\rangle \alpha + |\Pi_{out}\rangle, \quad \text{for } x > x_M \quad (F.7)$$

By matching the values and the derivatives of inner and outer solutions at $x = x_M$, we obtain the coefficients C and α . The latter coefficient must be equal to

$$\alpha = \langle j | \hat{V} | X + \chi \rangle, \quad (F.8)$$

which should provide a good check on the numerical accuracy of the solution.

To compute $GV|\chi\rangle$ with a given regular function $|\chi\rangle$ for positive energies, we can proceed just as for negative energies. Defining

$$|\Xi(x)\rangle = GV|\chi(x)\rangle, \quad (F.9)$$

we obtain

$$\left[\frac{d^2}{dx^2} + \frac{2}{x} \frac{d}{dx} - \frac{L(L+1)}{x^2} + q^2 - V(x) \right] \Xi(x) = V(x)\chi(x) \quad (F.10)$$

where $\Xi(x)$ must be regular, and at $x \geq R$ it must be proportional to $\hat{h}_L^{(+)}(qx)$.

$$|\Xi(x)\rangle \xrightarrow{x > R} |\hat{h}_L^{(+)}(qx)\rangle C \quad (F.11)$$

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For a coupled state, $|\hat{h}^{(+)}\rangle$ is a 2×2 diagonal matrix and C is a 2×1 row vector. We define the inner homogeneous solution Ξ_{in}^H that is regular ($x < x_M$), and the outer homogeneous solution Ξ_{out}^H for $x > x_M$ that becomes equal to $h_L^{(+)}(qx)$ at $x > R$. Using the inner and outer particular solutions $\Pi_{in,out}$ already defined in Eq.(F.5), we find

$$|\Xi(x)\rangle = |\Xi_{in}^H\rangle d + |\Pi_{in}\rangle, \quad \text{for } x < x_M \quad (\text{F.12})$$

$$|\Xi(x)\rangle = |\Xi_{out}^H\rangle C + |\Pi_{out}\rangle, \quad \text{for } x > x_M \quad (\text{F.13})$$

to be the solution of Eq.(10). For coupled states, both $|\Xi_{in}^H\rangle$ and $|\Xi_{out}^H\rangle$ are 2×2 matrix functions, and C and d are 2×1 row vectors. By matching smoothly the inner and outer solutions at $x = x_M$, we obtain the coefficients C and d which are complex in general. The coefficient C plays an important role in calculating the breakup amplitude.

Appendix G Analytic property of A_{α}

In order to solve our key equation (5.15)

$$A_{\alpha} = M_{\alpha} + S_{\alpha} N_{\alpha\alpha} A_{\alpha}, \quad (\text{G.1})$$

we must know the analytic property of each term. We follow the method of Larson and Hetherington²²). First, we define Property A and Property K. A function $f(p)$ will be said to have Property A if it is analytic along the real axis except a square-root branch point at the physical breakup threshold.

We have to deal with the integrals of the form

$$\xi(p) = \int_0^{\infty} dp' K(p,p') \eta(p'). \quad (\text{G.2})$$

The kernel will be said to have Property K if it takes the form of the Faddeev kernel,

$$K(p,p') = \int_{-1}^1 du P_{\gamma}(u) \frac{\rho(p,p';u)}{ME/\hbar^2 - p^2 - p'^2 - pp'u + i\epsilon} \quad (\text{G.3})$$

where $\rho(p,p';u)$ is analytic, and it has the same symmetry property as $\eta(p')$ when $p \rightarrow -p'$.

From Fig.13, we see that there are four critical points where $\xi(p)$ might become singular, even if $\eta(p)$ has Property A. These points are numbered 1, 2, 3 and 4 in Fig. 13. The locations 1 and 3 are where two logarithmic singularities join together, and the locations 2 and 4 are where the logarithmic singularities osculates the square-root branch point. Nevertheless, Larson and Hetherington²²⁾ have shown that if $\eta(p)$ is of Property A and if the kernel $K(p,p')$ has the Property K, then $\xi(p)$ also has Property A. We shall utilize this characteristic feature of the Faddeev equation fully in this appendix.

Our purpose here is to demonstrate that the solution $A_\alpha = A_\alpha(p)$ of Eq.(G.1) has Property A. The outline of our proof is as follows. First, we argue that Eq.(G.1) is the Faddeev equation in our representation, in that it has the Faddeev kernel (as we have shown in Appendix C). As has been shown by Faddeev, an iterated form of the kernel meets the Fredholm conditions. Thus, as in ref.15, we maintain that the analytic property of A_α is determined by that of each iteration of Eq.(G.1). Therefore, all that we have to show is that all kernels in M_α as well as in $S N_{\alpha\alpha}, A_{\alpha\alpha}$, are of Property K, and the inhomogeneous term M_α is of Property A. Then it follows automatically that the solution A_α has Property A.

Let us look at the perturbation series in W_α of the inhomogeneous term M_α . (See, section 5).

$$M_\alpha = \langle \tau_{\alpha\alpha}^F | Q | \alpha_0 \phi_d \chi \rangle + \sum_{m=1}^{\infty} S_{\alpha\alpha}^{(W)} \langle \tau_{\alpha\alpha}^F | Q | F_{\alpha\alpha}, z_{\alpha\alpha}^{(m)} \rangle \quad (G.4)$$

where

$$|z_{\alpha\alpha}^{(1)}(x)\rangle = W_{\alpha\alpha} (F_{\alpha\alpha} | Q | \alpha_0 \phi_d \chi \rangle \quad (G.5)$$

and

$$|z_{\alpha\alpha}^{(m)}(x)\rangle = W_{\alpha\alpha} S_{\alpha\alpha}^{(W)} (F_{\alpha\alpha} | Q | F_{\alpha\alpha}, z_{\alpha\alpha}^{(m-1)} \rangle \quad (m \geq 2) \quad (G.6)$$

The zero-th order term of M_α , i.e. $\langle \tau_{\alpha\alpha}^F | Q | \alpha_0 \phi_d \chi \rangle$, obviously has Property A. This is so because the bound state pole p_d lies above p_c (See, Fig.13), and because $|\tau_{\alpha\alpha}\rangle$ is actually a function of q rather than p (see Table 1).

In Appendix C, we have shown that $(F_{\alpha\alpha} | Q | F_{\alpha\alpha}, z_{\alpha\alpha} \rangle$ is given by Eq.(C.2).

$$(F_{\alpha\alpha} | Q | F_{\alpha\alpha}, z_{\alpha\alpha} \rangle = \sum_{L O S Y} C_{\alpha\alpha}^Y(p,p') [X_{L\alpha}^Y(p,p';x) + A_{\alpha\alpha}(q') Y_L^Y(p,p';x)]. \quad (G.7)$$

Here both $X_{L\alpha}^Y(p, p'; x)$ and $Y_L^Y(p, p'; x)$ have the kernel

$$\mathcal{K}(p, p'; x, x') \equiv \int_{-1}^1 du P_Y(u) \hat{j}_L(\lambda x) x'^2 \hat{j}_L(\lambda' x') \quad (G.8)$$

so that

$$X_{L\alpha}^Y(p, p'; x) = \int_0^R dx' \mathcal{K}(p, p'; x, x') [Z_\alpha(q'x') - A_\alpha(q') \hat{h}_L^{(+)}(q'x')] \quad (G.9)$$

and

$$Y_L^Y(p, p'; x) = \int_0^\infty dx' \mathcal{K}(p, p'; x, x') \hat{h}_L^{(+)}(q'x') \quad (G.10)$$

(See, Eqs. (C.7), (C.8) and (C.9) and also Eq. (C.13)). When $p' \rightarrow -p'$, the coefficient $C_{\alpha\alpha}^Y(p, p')$ changes its phase by $(-)^{b+b'+1} = (-)^{\gamma+\ell'+1}$ (See, Eqs. (C.5) and (C.6)). When $p' \rightarrow -p'$ is accompanied by $u \rightarrow -u$ in $\mathcal{K}(p, p'; x, x')$, λ and λ' remain unchanged (See Eq. (C.10)) while $P_Y(u)$ receives the phase factor $(-)^Y$. Therefore, $\mathcal{K}(p, p'; x, x')$ changes its sign by $(-)^Y$ under $p' \rightarrow -p'$. Thus, $C_{\alpha\alpha}^Y$ altogether gets the factor $(-)^{\ell'+1}$. The function $|Z_\alpha(q, x)\rangle$ (and therefore its asymptotic form $A_\alpha(q) \hat{h}_L^{(+)}(qx)$) is a function not only of q but also of p . Its asymmetry property under $p \rightarrow -p$ can be seen from Eqs. (G.5) and (G.6). When we change p to $-p$ there, $|Z_\alpha\rangle$ receives the factor $(-)^{\ell'+1}$ (W_α is an operator dependent only on q and hence does not change by $p \rightarrow -p$). Therefore, $|Z_\alpha\rangle$ changes its sign by $(-)^{\ell'+1}$ under $p' \rightarrow -p'$. This proves the Property K for all integrals involved in Eq. (G.4). Since $\langle \tau_{\alpha\alpha}^F | Q | \alpha_{\alpha\alpha} \phi_d \chi \rangle$ has Property A, and the kernels are of Property K, it follows that $M_{\alpha\alpha}$ is of Property A.

The kernels of the perturbation series of $N_{\alpha\alpha}$ have the same analytic structure of those of $M_{\alpha\alpha}$, and hence they all are of Property K. Since $M_{\alpha\alpha}$ has Property A, it follows that each iterate of Eq. (G.1) is of Property A. This completes the proof that $A_{\alpha\alpha}$ has Property A.

We point out that $A_\alpha(p)$, besides having Property A, should become zero as $p \rightarrow 0$. This can be demonstrated explicitly by integrating Eqs. (C.20) and (C.21) over p' near $p = 0$.

Appendix H Method of acceleration

In solving a linear integral equation

$$\phi = f + K\phi \quad (H.1)$$

in the iterative way

$$\phi = 1 + K + K^2 + K^3 + \dots \quad (\text{H.2})$$

the convergence of the series is governed by $||K||$. If it is larger (less) than unity, the series (H.2) diverges (converges). Conversely, it may be possible to obtain a faster convergence or even enlarge the convergence radius if we introduce a different kernel for solving the same equation (H.1). Thus, we have proposed the method of acceleration¹⁰⁾.

In this method, Eq.(H.1) is expressed with a parameter α as

$$\phi = (1 + \alpha K) \frac{1}{1 - T(\alpha)} f, \quad (\text{H.3})$$

where $T(\alpha)$ is defined by

$$T(\alpha) = (1 - \alpha)K + \alpha K K. \quad (\text{H.4})$$

Since Eq.(H.3) is written as

$$\phi = (1 + \alpha K) \frac{1}{(1 - K)(1 + \alpha K)} f = \frac{1}{1 - K} f, \quad (\text{H.5})$$

the iterative solution of Eq.(H.3)

$$\phi = (1 + \alpha K) (1 + T(\alpha) + T(\alpha)^2 + \dots) f \quad (\text{H.6})$$

should yield the solution of Eq.(H.1) when $||T(\alpha)|| < 1$. The merits of this method are two fold. (i) By a judiciously chosen value of α , we may be able to get a faster convergence. In practice, with increasing number of terms in the iterative series (H.2), the errors accumulate inevitably in the course of computations. On the other hand, if we get a faster convergence by the series (H.6), the accumulated error will be smaller. This is very important point to make the numerical result more accurate. In ref.10, we have demonstrated some examples showing the effectiveness of the method of acceleration. In fact, this method was indispensable in our 18 channel triton calculation¹⁷⁾. (ii) Another merit is that we can enlarge the radius of convergence. We demonstrate this point in this appendix, taking K as a constant rather than an operator as in Eq.(H.1). This is to aid understanding the method of acceleration. If we write this constant as x , the iterative solution of the linear equation

$$u = 1 + xu \quad (\text{H.7})$$

is given by

$$u = 1 + x + x^2 + \dots \quad (\text{H.8})$$

This series converges only if $||x|| < 1$. On the other hand, if we apply the method of acceleration, u is expressed as

$$u = (1 + \alpha x) \frac{1}{1 - [(1 - \alpha)x + \alpha x^2]} \quad (\text{H.9})$$

If we write

$$t(\alpha) = (1 - \alpha)x + \alpha x^2, \quad (\text{H.10})$$

then the iterative series

$$u = (1 + \alpha x) (1 + t(\alpha) + t(\alpha)^2 + \dots) \quad (\text{H.11})$$

converges if

$$|(1 - \alpha)x + \alpha x^2| < 1,$$

or in other words, if

$$-1 < (1 - \alpha)x + \alpha x^2 < 1. \quad (\text{H.12})$$

This condition is expressed as the relation between α and x as

$$\begin{aligned} x < 0; & -\frac{1}{x} > \alpha > -\frac{x+1}{x(x-1)} \\ 1 > x > 0; & -\frac{1}{x} < \alpha < -\frac{x+1}{x(x-1)} \\ x > 1; & -\frac{1}{x} > \alpha > -\frac{x+1}{x(x-1)}. \end{aligned} \quad (\text{H.13})$$

Therefore, we can extend the region of convergence to any value of x , although the suitable region of α becomes smaller with increasing $|x|$.

The minimum of $-(x+1)/x(x-1)$ is at $x = 1/\sqrt{3}$, where $-(x+1)/x(x-1) = 3 + 2\sqrt{3}$ and $-1/x = -\sqrt{3}$. Therefore, for $-1 < x < 1$, the value of $\alpha = 1$ is in the region of convergence given by (H.13) for the series (H.11).

In the region $0 < x < 1$, the series (H.11) for any value of α converges faster than the series (H.8) since $(1 - \alpha)x + \alpha x^2 < x$ is satisfied as an identity.

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Formulation of $n-d$ Elastic and Breakup Reactions

| α | p-interval | $ u_{\alpha}\rangle$ | $ \tau_{\alpha}\rangle$ | |
|----------|---------------------|-----------------------------|--|---------|
| $1S_0$ | $p_C < p < \bar{p}$ | $- \psi\rangle$ | $\frac{\lambda}{1-\lambda}\langle\psi V$ | Closed |
| | $0 < p < p_C$ | $- \hat{\omega}\phi\rangle$ | $\frac{1}{D}\langle j V\hat{\omega}$ | Breakup |

Table 1

The unperturbed part in Γ of Eq.(5.11).

| α | p-interval | W_{α} | |
|---------------|-----------------------|--|------------------|
| $1S_0$ | $p_C < p < \bar{p}$ | $(\omega - 1)$ | Closed |
| | $\bar{p} < p$ | GV | Closed |
| | $0 < p < p_C$ | $(\hat{\omega} - 1)$ | Closed |
| $3S_1 + 3D_1$ | $0 < p (q \neq iq_d)$ | $GV - \phi_d\rangle \frac{1}{q^2 + q_d^2} \langle \phi_d V$ | Closed + Breakup |
| | $q = iq_d$ | $(\omega - 1) - P(q)V$ | Closed* |
| Others | $0 < p$ | GV | Closed + Breakup |

Table 2

The operator W_{α} in the perturbational part in Γ of Eq.(5.11).* For $P(q)$, See Appendix B.

- Fig.1 The diagram representing $G_0 t$.
- Fig.2 Diagrammatic representation of the Faddeev equation (2.8). The diagram on the left hand side represents the function $|\phi\rangle$. The incident deuteron is depicted by the heavy line, at the open end of which we suppose $|\phi_d\rangle$ or $\langle\phi_d|$ is always attached. The first term on the right hand side is for the incident wave $|\phi_d j\rangle$.
- Fig.3 The spring shaped curve represents the operator Γ .
- Fig.4 Diagrammatic representation of the relation $G_0 t = |\phi_d\rangle G_0 \langle\phi_d| V + \Gamma$. The vertical dashed line in the first term on the right hand side of the diagram represents V .
- Fig.5 The relation (3.9), i.e., $|F\rangle = |j\rangle + G_0 \langle\phi_d| \bar{V} Q |\phi\rangle$ is depicted. The elastic component $|F\rangle$ is represented by the square on the left hand side.
- Fig.6 The elastic and non-elastic decomposition of $|\phi\rangle$ is represented by the first and the second diagram, respectively, on the right hand side.
- Fig.7 The decompositon of Γ , Eq.(5.12), into the unperturbed (separable) term and the perturbation W is depicted by the first and the second diagram, respectively, on the right hand side. The right-half-circle means $|F_{\alpha} \nu\rangle$ and the left-half-circle does $\langle\tau_{\alpha} F|$. The virthical line in the second diagram represents $|F_{\alpha}\rangle W_{\alpha} \langle F_{\alpha}|$.
- Fig.8 Diagrammatic representation of the operator $(1 - WQ)^{-1}$ on the left hand side expanded into the perturbation series on the right hand side.
- Fig.9 The matrix element $A = \langle\tau F|Q|\rho\rangle$ of Eq.(5.14) is illustrated for the case when $|\rho\rangle$ is equal to $|\phi\rangle$.
- Fig.10 The matrix element $M = \langle\tau F|Q(1 - WQ)^{-1}|\phi_d \chi\rangle$ of Eq.(5.16) is pictured. The wavy line on the right indicates the interaction in $|\chi\rangle$.
- Fig.11 Diagrammatic representation of the kernel N in Eq.(5.15), $N = \langle\tau F|Q(1 - WQ)^{-1}|F\nu\rangle$.
- Fig.12 Illustration of Eq.(5.13) for the case when $|\rho\rangle$ is equal to $|\phi\rangle$.
- Fig.13 The contours of the logarithmic singularities is $Y_L^Y(p, p'; x)$ of Eq.(C.23). The curves $p' = \mu$ and $p' = -\nu$ correspond to $u_0 = -1$ while the curve $p' = \nu$ corresponds to $u_0 = +1$. Within the crescent shaped region, $-1 < u_0 < 1$, and $Y_L^Y(p, p'; x)$ is complex with the imaginary part given by Eq.(C.31). The bound state pole is indicated by p_d . The numbers 1, 2, 3 and 4 show the locations where two logarithmic singularities join together (1 and 3) and where the logarithmic singularity osculates with the square-root branch point(2 and 4).



Fig. 1

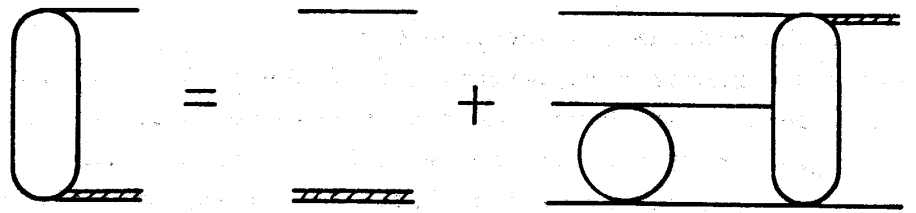


Fig. 2

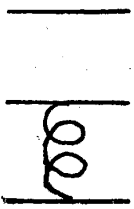


Fig. 3

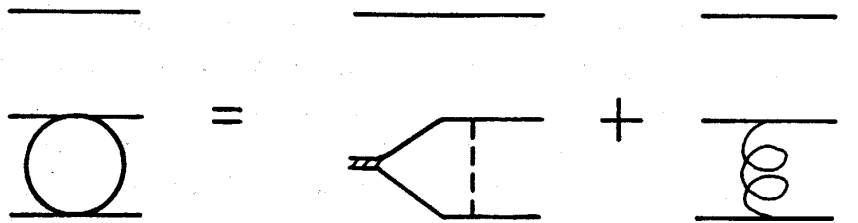


Fig. 4

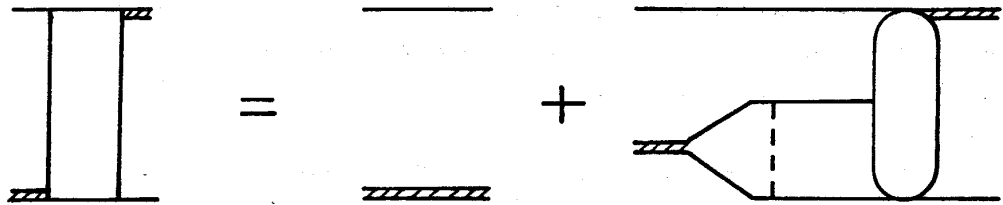


Fig. 5

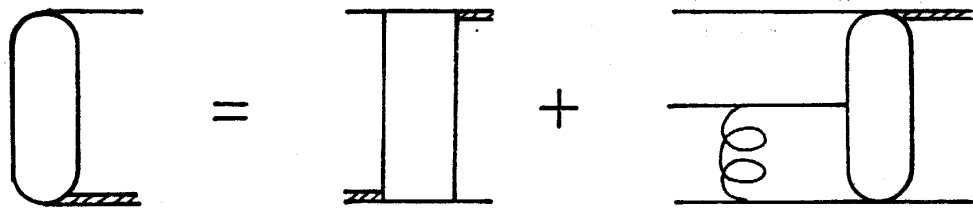


Fig. 6

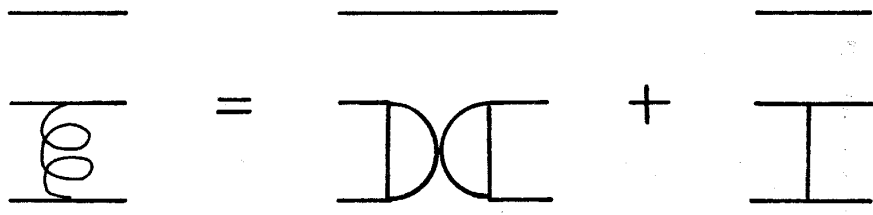


Fig. 7

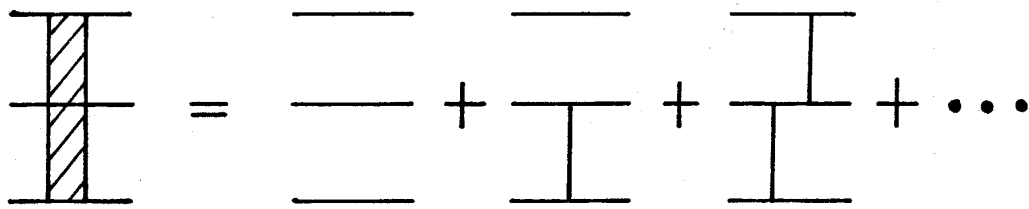


Fig. 8

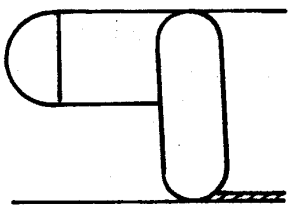


Fig. 9

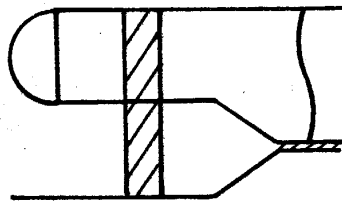


Fig. 10

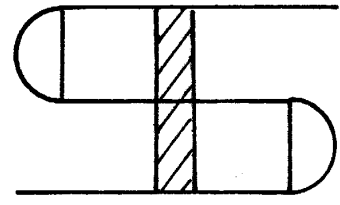


Fig. 11

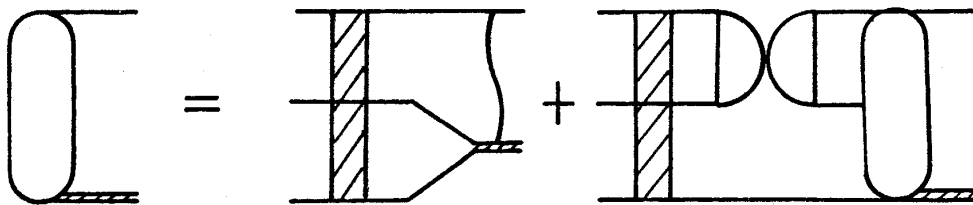


Fig. 12

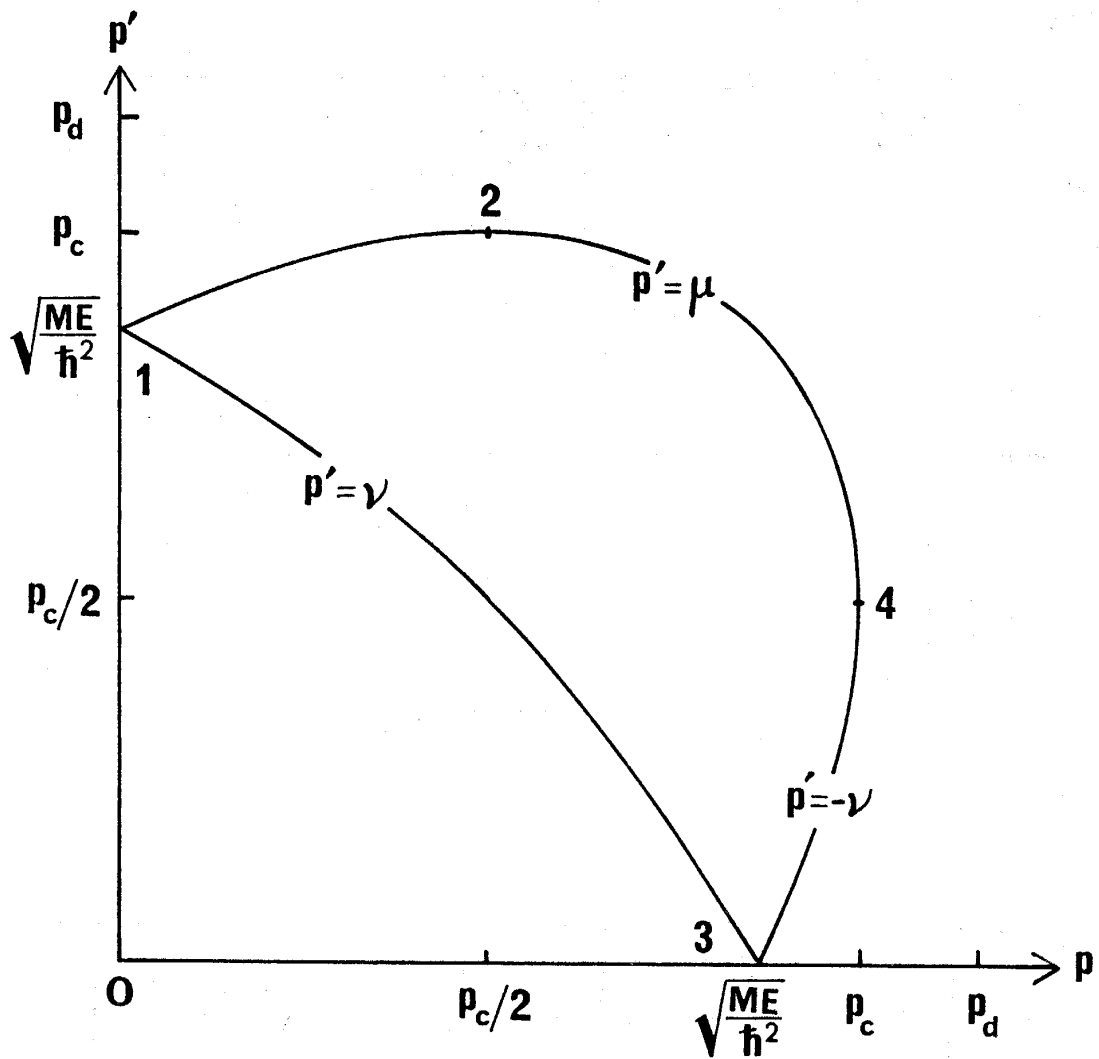


Fig. 13