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## A symmetric theory of collisions

B. G. Giraud and M. A. Nagarajan (\*)

Division de la Physique, Service de Physique Théorique, CEN Saclay, B.P. 2, 91190 Gif sur Yvette, France

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**Résumé.** — Au lieu des matrices  $T_{\beta\alpha}$  usuelles, dont la définition varie quand les partitions liées aux voies  $\alpha$  et  $\beta$  changent, il est possible de définir un opérateur  $T$  unique. Les amplitudes de transition physiques deviennent alors des résidus de pôles pour des éléments de matrice bien choisis de cet opérateur  $T$ . Les problèmes soulevés par le mouvement du centre de masse, le principe de Pauli et l'alternative post-prior sont simplifiés par la nature symétrique de cet opérateur  $T$ . La théorie peut être reliée à un principe variationnel afin de faciliter le calcul pratique des éléments de matrice  $T$ .

**Abstract.** — Instead of the usual transition operators  $T_{\beta\alpha}$ , whose definitions change when the partitions corresponding to  $\alpha$  and/or  $\beta$  change, it is possible to define a unique  $T$ -operator. The physical transition amplitudes are then recovered as residues of poles of specific matrix elements of the  $T$ -operator. Problems raised by the centre-of-mass motion, the Pauli principle and the post-prior alternative are simplified by the symmetry of the  $T$ -operator. The theory can be related to a variational principle in order to allow for practical calculations of the matrix elements of the  $T$ -operator.

1. **Introduction.** — Familiar theories [1] of rearrangement collisions for a transition from a channel  $\alpha$  to a channel  $\beta$  consist, as a first step, in splitting the total nucleus-nucleus interaction  $V = \sum_{i < j} V_{ij}$  in the form  $U_\alpha + V_\alpha$  where  $U_\alpha$  is the sum of the binding interactions of the incoming projectile and the target and  $V_\alpha$  is the residual (prior) interaction. A similar splitting of  $V$  into  $U_\beta$  and  $V_\beta$ , the binding and post interactions respectively relevant to the final channel, is also considered. A second step of the theory consists in defining the post (prior) transition operator

$$T_{\beta\alpha} = V_\beta(V_\alpha) + V_\beta G^{(+)} V_\alpha,$$

where  $G^{(+)}$  is the total Green's function

$$G^{(+)} = (E - H + i\epsilon)^{-1}.$$

This is clearly a theory which would gain some elegance if the channel labels and partitions do not need to be introduced explicitly. For an attempt in this direction, one may note that both  $V_\alpha$  and  $V_\beta$  are equivalent to  $(E - H)$  when they act upon states

of their respective channels at the on-shell energy  $E$ . Then  $T_{\beta\alpha}$  reduces [2] to

$$(E - H) + (E - H)(E - H + i\epsilon)^{-1}(E - H),$$

which appears more symmetric, although a little confusing.

It is tempting to consider the global  $T$ -operator  $T = V + VG^{(+)}V$ , where only the total interaction appears. Such an operator is defined without the need of any preliminary channel specification, and it is felt that it may contain all the information relevant to the various transition operators  $T_{\beta\alpha}$ . It has indeed been shown by Weinberg [3] that the calculation of the total Green's function  $G^{(+)}$  yields a complete solution of the many-body problem and it is seen that the information contained in  $T$  should be as complete as that given by  $G$ .

It should be pointed out that the point raised in the preceding paragraph has been considered in great detail by Lehmann, Symanzik and Zimmermann [4] (LSZ) in the description of interacting fields. Non-relativistic versions of the LSZ formulae have been discussed by Redmond and Uretsky [5] and Ballot and Becker [6]. A many particle scattering in second quantized representation has been derived by Villars [7].

(\*) Daresbury Laboratory, Daresbury, Warrington WA4 4AD, U.K.

In the particular case of the three-body problem, the singularities of the global  $T$ -operator have been discussed by Fadeev [8] and by Osborn and Kowalski [9]. The effect of exchange has been discussed by Benze and Redish [10].

In this paper, our purpose is to show that the global  $T$ -operator provides a complete theory of collisions. In section 2, we discuss the symmetry properties of the global  $T$ -operator. We also define the antisymmetrized matrix elements of this  $T$ -operator in the barycentric frame. The vertex functions are defined in section 3 for the various subsystems which can form bound states. The relation between the global  $T$ -operator and the channel  $T$ -operators is discussed in section 4. We rederive in section 5, with a new approach, the familiar result that the matrix elements of the channel  $T$ -operator are residues of the matrix elements of the global  $T$ -operator. The nature of the residues and the method of their evaluation are discussed in section 6. This is illustrated in section 7, by a specific example. In section 8, we present a variational formalism for the elements of the global  $T$ -operator. The final section, section 9, presents the conclusions and summary of our work.

**2. Symmetry properties of the global  $T$ -matrix formalism.** — The  $N$ -nucleon Hamiltonian  $H = K + V$  is the usual sum of kinetic energies and two-body potentials

$$H = \sum_{i=1}^N K_i \left\{ \begin{array}{l} - K_{\text{cm}} \\ + \frac{1}{2} M \omega^2 R_{\text{cm}}^2 \end{array} \right\} + \sum_{i>j=1}^N V_{ij}, \quad (2.1)$$

modified, however, by the subtraction of the centre-of-mass kinetic energy or the addition of a centre-of-mass harmonic binding. The first choice for the modification makes  $H$  a pure internal Hamiltonian. The second choice adds to this internal Hamiltonian a harmonic oscillator for the centre-of-mass.

In both cases the centre-of-mass is decoupled from the physical (internal) dynamics. The second choice may be preferable, for the physical spectrum is shifted by discrete amounts  $(\frac{3}{2} + n)\hbar\omega$ ,  $n = 0, 1, \dots, \infty$ , while the first case makes the spectrum of  $H$  in the  $N$ -body space equal to the physical spectrum, but with an infinite degeneracy due to the spectator centre-of-mass states.

Whatever the choice made in eq. (2.1) the Hamiltonian contains at most two-body operators and is symmetric. We call  $V$  the sum  $\sum_{i>j} V_{ij}$  and  $K$  the rest.

We define the bare and complete resolvents

$$G_0 = (W - K)^{-1}, \quad G = (W - H)^{-1}, \quad (2.2)$$

and the global  $T$ -operator

$$T(W) = V + VGV, \quad (2.3)$$

where  $W$  is a parametric energy. As long as  $W$  is complex the resolvents are well defined and  $T$  obeys the usual integral equation

$$T = V + VG_0 T. \quad (2.4)$$

It is obvious that all these operators  $V, K, G_0, G$  and  $T$  are symmetric.

We now consider the kets  $|\mathbf{k}_1 \dots \mathbf{k}_N\rangle$  defined by the wave function

$$\langle \mathbf{r}_1 \dots \mathbf{r}_N | \mathbf{k}_1 \dots \mathbf{k}_N \rangle = \pi^{-3/4} \lambda^{-3/2} \times \\ \times \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \dots + \mathbf{k}_N \cdot \mathbf{r}_N)] \exp - \frac{R_{\text{cm}}^2}{2\lambda^2}, \quad (2.5)$$

with the constraint  $\sum_i \mathbf{k}_i = 0$  and  $\lambda = (\hbar/M\omega)^{1/2}$ . It is trivial to check that  $|\mathbf{k}_1 \dots \mathbf{k}_N\rangle$  is an eigenstate of  $K$ . The eigenvalue is the usual kinetic energy, increased by  $\frac{3}{2}\hbar\omega$  if necessary. We also notice that *a priori* nothing prevents to take  $\mathbf{k}_1 \dots \mathbf{k}_N$  as complex vectors. The point of interest is that no matrix element of  $K, V, H, \dots, T$ , nor any operator function of these operators will ever connect  $|\mathbf{k}_1 \dots \mathbf{k}_N\rangle$  to any state with a different centre-of-mass wave packet. The problem of Galilean invariance is thus *a priori* solved if matrix elements  $\langle \mathbf{k}'_1 \dots \mathbf{k}'_N | T | \mathbf{k}_1 \dots \mathbf{k}_N \rangle$  are correctly evaluated.

In the following we consider antisymmetrized matrix elements

$$\tilde{T}(\mathbf{k}', \mathbf{k}) \equiv \langle \mathbf{k}'_1 \dots \mathbf{k}'_N | \mathcal{A} T \mathcal{A} | \mathbf{k}_1 \dots \mathbf{k}_N \rangle, \quad (2.6)$$

where  $\mathbf{k}$ , resp.  $\mathbf{k}'$ , is a short notation for  $(\mathbf{k}_1 \dots \mathbf{k}_N)$ , resp.  $(\mathbf{k}'_1 \dots \mathbf{k}'_N)$  and the antisymmetrizer  $\mathcal{A}$  is defined by

$$\langle \mathbf{r}_1 \dots \mathbf{r}_N | \mathcal{A} | \mathbf{k}_1 \dots \mathbf{k}_N \rangle = (N!)^{-1/2} \times \\ \times \sum_{\mathcal{P}} (-)^{\mathcal{P}} \langle \mathcal{P}(\mathbf{r}_1 \dots \mathbf{r}_N) | \mathbf{k}_1 \dots \mathbf{k}_N \rangle, \quad (2.7)$$

the permutation  $\mathcal{P}$  exchanging the coordinates  $\mathbf{r}_1 \dots \mathbf{r}_N$ . It is clear that the consideration of  $\tilde{T}(\mathbf{k}', \mathbf{k})$  takes fully into account the Pauli principle and eq. (2.6) could as well be written in second quantization. It will be shown in the next sections that the singularities of this highly symmetric function,  $\tilde{T}(\mathbf{k}', \mathbf{k})$ , are easily related to physical scattering amplitudes between fermion clusters.

**3. Vertex functions.** — It is not uncommon that the spectrum of  $H$  contains, below continuous thresholds, discrete eigenvalues  $E_n^N$  corresponding to bound states  $\varphi_n^N$  of  $N$  nucleons. Since  $T = V + V(W - H)^{-1} V$ , the behaviour of  $\tilde{T}(\mathbf{k}', \mathbf{k})$ , when  $W \rightarrow E_n^N$  for an arbitrary choice of  $\mathbf{k}$  and  $\mathbf{k}'$ , is obviously that of a simple pole. The vertex function is then defined by the residue

$$N! \langle \mathbf{k}' | V | \varphi_n^N \rangle \langle \varphi_n^N | V | \mathbf{k} \rangle = \\ = \lim_{W \rightarrow E_n^N} (W - E_n^N) \tilde{T}(\mathbf{k}', \mathbf{k}). \quad (3.1)$$

Alternately a contour integral in the  $W$ -plane about the  $E_n^N$  pole gives the same residue. This question of vertex functions has received already much attention in the literature and we shall consider these vertex functions as known in the next sections.

More precisely, in order to investigate a collision of two nuclei adding up to  $N$  nucleons, we shall assume that all vertex function for  $N' < N$  have been tabulated in advance, or can be derived (at least approximately) by suitable approximations to the calculation of  $\tilde{T}(\mathbf{k}', \mathbf{k})$  in eq. (3.1). In the same way, we assume that all necessary energies  $E_n^{N'}$  are known when  $N' < N$  (of course the poles of  $\tilde{T}(\mathbf{k}', \mathbf{k})$  may have to be shifted by  $\frac{3}{2} \hbar \omega$  to recover the physical energies, but this kind of precaution will be understood in the following).

**4. Connection with channel  $T$ -matrices.** — We are interested in a transfer collision with *two-body* initial channel  $\alpha$  with nuclei  $A' A''$  and final channel  $\beta$  with nuclei  $B' B''$ . The total physical energy is  $E = E_\alpha + E_m^\alpha$ , where  $E_\alpha$  is the energy available in the channel above the threshold energy  $E_m^\alpha = E_{m'}^{A'} + E_{m''}^{A''}$ , sum of the self-energies of the nuclei in their eigenstates labelled by  $m'$  and  $m''$ . In the same way  $E = E_\beta + E_n^\beta$ , where  $E_\beta$  is the kinetic energy available in the final channel and  $E_n^\beta$  the self-energy of the channel.

The nucleons numbered 1 to  $A'$  are considered arbitrarily to belong to nucleus  $A'$  and those from  $(A' + 1)$  to  $N$  to nucleus  $A''$ . We split  $V$  into  $V_\alpha$  and  $U_\alpha$ , where  $V_\alpha$  contains all potentials  $V_{ij}$  such as  $i > A'$  and  $j \leq A'$ . In other words  $V_\alpha$  is the prior interaction and  $U_\alpha$  is that interaction considered to be internal to the initial channel.

In the same way for the channel  $\beta$  we give labels 1 to  $B'$  to nucleons inside nucleus  $B'$  and labels  $(B' + 1)$  to  $N$  to nucleons inside  $B''$  and we obtain the post potential  $V_\beta$  and internal potential  $U_\beta$ .

A straightforward but slightly tedious manipulation of eq. (2.3) gives the *two potential identity* [11]

$$\begin{aligned} T(W) &= \Omega_\beta^\dagger(W) T_{\beta\alpha}^{\text{prior}}(W) \Omega_\alpha(W) + U_\alpha \Omega_\alpha(W) \\ &= \Omega_\beta^\dagger(W) T_{\beta\alpha}^{\text{post}}(W) \Omega_\alpha(W) + \Omega_\beta^\dagger(W) U_\beta, \end{aligned} \quad (4.1)$$

where

$$\begin{aligned} \Omega_\alpha(W) &= 1 + (W - K - U_\alpha)^{-1} U_\alpha, \\ \Omega_\beta^\dagger(W) &= 1 + U_\beta(W - K - U_\beta)^{-1}, \\ T_{\beta\alpha}^{\text{prior}} &= V_\alpha + V_\beta(W - H)^{-1} V_\alpha, \\ T_{\beta\alpha}^{\text{post}} &= V_\beta + V_\beta(W - H)^{-1} V_\alpha. \end{aligned} \quad (4.2)$$

It may be pointed out that, while the limit of eq. (4.1) when  $W \rightarrow E + i\epsilon$  demands precautions because  $\Omega_\beta^\dagger$ ,  $T_{\beta\alpha}$  and  $\Omega_\alpha$  may be simultaneously singular, this eq. (4.1) is a strict identity as long as these operators are non singular ( $W$  complex). One recognizes then that  $\Omega_\alpha$ ,  $\Omega_\beta^\dagger$  become Möller operators on the energy shell and  $T_{\beta\alpha}^{\text{prior}}$ ,  $T_{\beta\alpha}^{\text{post}}$  are the usual  $T$ -operators relating

to the specific partitions induced by the above description of the channel  $\alpha$  and  $\beta$ .

If now we consider in channel  $\beta$  a permutation  $\mathcal{P}$  different from the identity  $(^1)$ , let  $\bar{i}_1$  be the label of the particle replacing particle 1,  $\bar{i}_2$  that of the particle replacing particle 2 and so on. Assigning  $\bar{i}_1 \dots \bar{i}_{B'}$  to nucleus  $B'$  and  $\bar{i}_{B'+1} \dots \bar{i}_N$  to  $B''$ , we define new operators  $\bar{V}_\beta$ ,  $\bar{U}_\beta$ ,  $\bar{\Omega}_\beta^\dagger$ ,  $\bar{T}_{\beta\alpha}$  accordingly. It is clear that  $\bar{T}_{\beta\alpha}$  will give an exchange  $T$ -matrix element while  $T_{\beta\alpha}$  will give a direct process matrix element. Thus eq. (4.1) generalizes for each partition into

$$T(W) = \bar{\Omega}_\beta^\dagger(W) \bar{T}_{\beta\alpha}^{\text{prior}}(W) \Omega_\alpha(W) + U_\alpha \Omega_\alpha(W). \quad (4.3)$$

To conclude this section it can be stressed that the splitting of  $V$  into channel internal and residual interactions connects the global  $T$ -operator to the familiar Möller operators and  $T$ -operators relating to specific channels and partitions.

**5. Double pole singularities.** — Because of the symmetry of  $T$ , the number  $\tilde{T}(\mathbf{k}', \mathbf{k})$  also reads

$$\tilde{T}(\mathbf{k}', \mathbf{k}) = \sum_{\mathcal{P}} (-)^{\mathcal{P}} \langle \bar{\mathbf{k}}'_1 \dots \bar{\mathbf{k}}'_N | T | \mathbf{k}_1 \dots \mathbf{k}_N \rangle, \quad (5.1)$$

where we let now the permutations  $\mathcal{P}'$  exchange  $\mathbf{k}'_1 \dots \mathbf{k}'_N$  into  $\bar{\mathbf{k}}'_1 \dots \bar{\mathbf{k}}'_N$ . We will then study the singularities of the non antisymmetrized matrix elements  $T(\bar{\mathbf{k}}', \mathbf{k})$  occurring in the right-hand side of eq. (5.1).

We first study  $T(\mathbf{k}', \mathbf{k})$ , corresponding to the identity  $(^2)$  for  $\mathcal{P}'$ . With particle labels 1 to  $A'$  inside nucleus  $A'$  and labels  $(A' + 1)$  to  $N$  inside  $A''$ , we combine  $\mathbf{k}_1 \dots \mathbf{k}_{A'}$  into  $(A' - 1)$  Jacobi momenta  $\kappa_{A'}$  internal to  $A'$ , then  $\mathbf{k}_{A'+1} \dots \mathbf{k}_N$  into  $(A'' - 1)$  Jacobi momenta  $\kappa_{A''}$  internal to  $A''$  and finally find a relative momentum  $\mathbf{k}_\alpha$  in the channel (the total momentum has already been constrained to vanish, see after eq. (2.5)). The ket  $|\mathbf{k}\rangle$  then reads  $|\kappa_\alpha \mathbf{k}_\alpha\rangle$  in an obvious short notation. A similar reduction of  $\mathbf{k}'_1 \dots \mathbf{k}'_{B'}$  and  $\mathbf{k}'_{B'+1} \dots \mathbf{k}'_N$  into Jacobi momenta defines as well a final channel momentum  $\mathbf{k}'_\beta$  and internal momenta  $\kappa'_\beta$ .

It is now convenient to consider  $T(\mathbf{k}', \mathbf{k})$  as a function of  $\kappa_\alpha$  and  $\mathbf{k}_\beta$  only, namely to freeze  $W$ ,  $\kappa_\alpha$  and  $\kappa'_\beta$ , and take advantage of eq. (4.1) to get the form

$$\begin{aligned} T(\mathbf{k}'_\beta, \mathbf{k}_\alpha) &\equiv T(\mathbf{k}', \mathbf{k}) = \\ &= \langle \kappa'_\beta \mathbf{k}'_\beta | (\Omega_\beta^\dagger T_{\beta\alpha}^{\text{post}} \Omega_\alpha + \Omega_\beta^\dagger U_\beta) | \kappa_\alpha \mathbf{k}_\alpha \rangle. \end{aligned} \quad (5.2)$$

According to eqs. (4.2) this also reads

$$\begin{aligned} T(\mathbf{k}'_\beta, \mathbf{k}_\alpha) &= \langle \kappa'_\beta \mathbf{k}'_\beta | \Omega_\beta^\dagger \times \\ &\times \{ U_\beta + T_{\beta\alpha}^{\text{post}} [1 + (W - E_\alpha - H_\alpha)^{-1} U_\alpha] \} | \kappa_\alpha \mathbf{k}_\alpha \rangle, \end{aligned} \quad (5.3)$$

(<sup>1</sup>) Notice, however, that rearrangement within a cluster is equivalent to an identity operation.

(<sup>2</sup>) Same footnote as for  $\mathcal{P}$ .

where  $E_\alpha = \hbar^2 k_\alpha^2 / 2 \mu_\alpha$ , in an obvious notation, is the kinetic energy available in the channel  $\alpha$  with the partition under consideration and  $H_\alpha$  is the corresponding internal Hamiltonian. With  $W$  complex nothing prevents us from adjusting  $\mathbf{k}_\alpha$  so that

$$(W - E_\alpha) \rightarrow E_m^\alpha,$$

the channel self-energy considered at the beginning of section 4. The residue of the pole is, obviously,

$$\begin{aligned} \lim (W - E_\alpha - E_m^\alpha) T(\mathbf{k}'_\beta, \mathbf{k}_\alpha) = \\ = \langle \kappa'_\beta \mathbf{k}'_\beta | \Omega_\beta^\dagger T_{\beta\alpha}^{\text{post}} | \varphi_m^\alpha \mathbf{k}_\alpha \rangle \langle \varphi_m^\alpha | U_\alpha | \kappa_\alpha \rangle, \\ k_\alpha \rightarrow [2 \mu_\alpha (W - E_m^\alpha) / \hbar^2]^{1/2}, \end{aligned} \quad (5.4)$$

where  $\varphi_m^\alpha$  is the product of the two bound-state wavefunctions  $\varphi_m^{\alpha'}$  and  $\varphi_m^{\alpha''}$  of the nuclei in the channel. Accordingly the vertex function  $\langle \varphi_m^\alpha | U_\alpha | \kappa_\alpha \rangle$  is the product of the vertex functions for the two nuclei,  $\langle \varphi_m^{\alpha'} | U_{\alpha'} | \kappa_{\alpha'} \rangle$  and  $\langle \varphi_m^{\alpha''} | U_{\alpha''} | \kappa_{\alpha''} \rangle$ .

We can stress here that i)  $W$  is complex, with a slight positive imaginary part and thus the physical limit has not yet been taken, then ii) the magnitude  $k_\alpha$  is positive, with a slight positive imaginary part, but the difference  $W - \hbar^2 k_\alpha^2 / 2 \mu_\alpha$  can be taken as a purely real, negative number close to  $E_m^\alpha$ , thus iii)  $\Omega_\alpha$  is having real energy denominators. The limit, eq. (5.4), thus disentangles the pole of  $\Omega_\alpha$  from the cuts of  $T_{\beta\alpha}$ .

A similar argument concerning the limit obtained with  $\mathbf{k}'_\beta$  gives the result

$$\begin{aligned} \lim (W - E'_\beta - E_n^\beta) (W - E_\alpha - E_m^\alpha) T(\mathbf{k}'_\beta, \mathbf{k}_\alpha) = \\ = \langle \varphi_n^\beta \mathbf{k}'_\beta | T_{\beta\alpha}^{\text{post}} | \varphi_m^\alpha \mathbf{k}_\alpha \rangle \langle \kappa_\beta | U_\beta | \varphi_n^\beta \rangle \langle \varphi_m^\alpha | U_\alpha | \kappa_\alpha \rangle, \\ k'_\beta \rightarrow [2 \mu_\beta (W - E_n^\beta) / \hbar^2]^{1/2}, \\ k_\alpha \rightarrow [2 \mu_\alpha (W - E_m^\alpha) / \hbar^2]^{1/2}. \end{aligned} \quad (5.5)$$

Here again  $k'_\beta$  has a slight positive imaginary part which can be adjusted so that the energy denominator induced in  $\Omega_\beta^\dagger$  by  $(W - \hbar^2 k'^2_\beta / 2 \mu_\beta - H_\beta)$  be real. The vertex function  $\langle \kappa_\beta | U_\beta | \varphi_n^\beta \rangle$  is again assumed to be known from section 3.

The two limits present in eq. (5.5) may be commuted and present *a priori* no difficulty other than technical. More important is the investigation of the limit of the right-hand side of eq. (5.5) when the positive imaginary part  $\varepsilon$  of  $W = E + i\varepsilon$ , with  $E$  the physical energy, is made to vanish. It is obvious that the vertex functions bring no difficulty and thus we concentrate on the  $T$ -matrix element. It reads, in a short notation

$$\begin{aligned} T(+i\varepsilon) = \langle \beta, n, \hat{k}'_\beta, (E - E_n^\beta + i\varepsilon)^{1/2} \times \\ \times | T_{\beta\alpha}(E + i\varepsilon) | \alpha, m, \hat{k}'_\alpha, (E - E_m^\alpha + i\varepsilon)^{1/2} \rangle, \end{aligned} \quad (5.6)$$

where  $\hat{k}'_\beta$  and  $\hat{k}'_\alpha$  indicate the orientations of  $\mathbf{k}'_\beta$  and  $\mathbf{k}_\alpha$ .

A crucial property of this number  $T(+i\varepsilon)$  is that it is a *completely on-shell* matrix element, as seen by the exact square root links between  $W$  and the complex lengths of  $\mathbf{k}'_\beta$  and  $\mathbf{k}_\alpha$ . On-shell matrix elements are

usually considered only for real values of the energy, but their analytic continuation away from the real axis should normally be possible in a non vanishing domain. We thus consider that there is sufficiently reasonable evidence that the limit of  $T(i\varepsilon)$  when  $\varepsilon \rightarrow 0$  is the desired physical amplitude [12].

To summarize this section we consider that the double limit, eq. (5.5), taken for  $W$  complex, and followed by the limit where  $W$  becomes real, is a way to extract physical amplitudes from the global  $T$ -matrix formalism.

**6. Sorting out of the residues.** — The argument leading to eq. (5.5) is mainly based on the identity, eq. (4.1), which leads to identification of the residue as a matrix element of  $T_{\alpha\beta}$ . Other identities like eq. (4.3) are available, however. It is important to check that different partitions in the particle labels do not lead to additional singularities modifying the interpretation of the residue of  $T(\mathbf{k}', \mathbf{k})$ .

Let  $\bar{i}_1, \dots, \bar{i}_B$  be a distinct <sup>(3)</sup> numbering for the nucleons of nucleus  $B'$  and  $\bar{i}_{B'+1} \dots \bar{i}_N$  the corresponding numberings for  $B''$ . For the given set of labels  $\mathbf{k}'_1 \dots \mathbf{k}'_N$  the reduction of  $\mathbf{k}'_{\bar{i}_1} \dots \mathbf{k}'_{\bar{i}_B}$  to Jacobi momenta  $\bar{\mathbf{k}}_{B'}$  and that of  $\mathbf{k}'_{\bar{i}_{B'+1}} \dots \mathbf{k}'_{\bar{i}_N}$  to  $\bar{\mathbf{k}}_{B''}$  define a new channel momentum  $\mathbf{k}'_\beta$ . It is trivial to see that in general  $\mathbf{k}'_\beta \neq \mathbf{k}_\beta$ . It is therefore in general possible not to bring simultaneously  $\mathbf{k}'_\beta$  and  $\mathbf{k}_\beta$  *on-shell* and thus the only residue occurring in the right-hand side of eq. (5.5) is indeed that shown by this eq. (5.5). This point is shown in more detail by the illustrative example of section 7.

A risk of wrong identification of the residue occurs also in relation with three-body channels. Let  $\gamma$  be such a channel, characterized by nuclei  $C'$ ,  $C''$  and  $C'''$  and the corresponding quantum numbers  $n'$ ,  $n''$ ,  $n'''$ , with the self-energy  $E_n^\gamma = E_n^{C'} + E_n^{C''} + E_n^{C'''}$ . Any partition  $\{i\}$  of nucleons  $1 \dots N$  between  $C'$ ,  $C''$ ,  $C'''$  defines internal Jacobi momenta  $\bar{\mathbf{k}}_{C'}$ ,  $\bar{\mathbf{k}}_{C''}$ ,  $\bar{\mathbf{k}}_{C'''}$  and channel relative momenta  $\bar{\mathbf{k}}_{C'C''}$  and  $\bar{\mathbf{k}}_{C'C'''}$ . It is trivial to check that, for a set of momenta  $\mathbf{k}'_1 \dots \mathbf{k}'_N$  which makes  $\mathbf{k}'_\beta$  *on-shell*, the momenta  $\bar{\mathbf{k}}_{C'C''}$  and  $\bar{\mathbf{k}}_{C'C'''}$  will in general not correspond to the situation where the three-body channel  $\gamma$  is *on-shell*. The residue in the right-hand side of eq. (5.5) has therefore no contribution from an identity such as the generalization of eq. (4.3) to three-body channels. The same argument and conclusion hold for channels  $\delta$  with more than three bodies. More details can be found in the illustrative example of section 7.

To summarize this argument the singularity of  $T(\mathbf{k}', \mathbf{k})$ , when this part of the global  $T$ -matrix element is made *on-shell* according to the limit used in eq. (5.5), is restricted in general to that transition  $T_{\beta\alpha}$  described by eq. (5.5). The key point of the argument

<sup>(3)</sup> Again here a distinct numbering means a true exchange between the channel nuclei.

is that the number of all other partitions and channels is in general *finite*. One can thus choose  $(\kappa'_\beta, \mathbf{k}'_\beta)$  and  $(\kappa_\alpha, \mathbf{k}_\alpha)$  so that all the other internal and channel momenta  $(\kappa'_\gamma, \mathbf{k}'_\gamma)$  and  $(\kappa_\gamma, \mathbf{k}_\gamma)$  resulting from the reduction to the other Jacobi momenta are off-shell.

It is now necessary to consider the other terms  $\langle \bar{\mathbf{k}}' | T | \mathbf{k} \rangle$  contained in  $\tilde{T}(\mathbf{k}', \mathbf{k})$ , eq. (5.1). The labels  $\mathbf{k}', \mathbf{k}$  of  $\tilde{T}$  being the same as those of its first term  $T(\mathbf{k}', \mathbf{k})$ , we use again the same reduction to Jacobi momenta and consider  $\tilde{T}$  as a function of the same  $\mathbf{k}'_\beta, \mathbf{k}_\alpha$  only. Again we consider the limit of

$$\mathcal{R} \equiv (W - E'_\beta - E_n^\beta)(W - E_\alpha - E_n^\alpha) \tilde{T}(\mathbf{k}'_\beta, \mathbf{k}_\alpha), \tag{6.1}$$

when  $\mathbf{k}'_\beta$  and  $\mathbf{k}_\alpha$  are made on-shell in the same way as in eq. (5.5). Let  $\mathcal{P}$  be the permutation of final momenta which characterizes a term  $\langle \bar{\mathbf{k}}' | T | \mathbf{k} \rangle$ . If one uses eq. (4.3) to analyse the behaviour of that term, it is clear that the permutation  $\mathcal{P}$  which leads to eq. (4.3) has to be equivalent to  $\mathcal{P}'$  if the resulting momenta  $(\bar{\mathbf{k}}'_\beta, \bar{\mathbf{k}}'_\beta)$  must remain  $\kappa'_\beta$  and  $\mathbf{k}'_\beta$ .

More precisely, since  $\mathcal{P}'$  exchanges momenta and  $\mathcal{P}$  exchanges the particles, the Jacobi and channel momenta are not changed when  $\mathcal{P}$  and  $\mathcal{P}'$  are equivalent. The term  $\langle \bar{\mathbf{k}}' | T | \mathbf{k} \rangle$  diverges therefore in the same way as the first term  $T(\mathbf{k}', \mathbf{k})$ . The corresponding residue then contains the same vertex functions and an on-shell matrix element of that exchange  $T$ -operator  $\bar{T}_{\beta\alpha}$  defined by the permutation  $\mathcal{P}$ .

On the other hand if  $\mathcal{P}$  and  $\mathcal{P}'$  are not equivalent, the channel and Jacobi momenta are those obtained by replacing  $\mathcal{P}'$  by the identity and  $\mathcal{P}$  by  $\mathcal{P}'^{-1} \mathcal{P}$ . It has already been seen that in general the new channel momentum  $\bar{\mathbf{k}}'_\beta$  is different from  $\mathbf{k}'_\beta$ . It thus cannot go on-shell simultaneously with  $\mathbf{k}'_\beta$ , and no contribution to the pole is found.

We have thus proved that in general the on-shell limit of  $\mathcal{R}$ , eq. (6.1) is

$$\lim \mathcal{R} = \langle \kappa'_\beta | U_\beta | \varphi_n^\beta \rangle \langle \varphi_n^\alpha | U_\alpha | \kappa_\alpha \rangle \sum_{\mathcal{P}} (-)^{\mathcal{P}} \bar{T}(+i\epsilon), \tag{6.2}$$

where  $\bar{T}(+i\epsilon)$  is the on-shell element of the  $T$ -operator defined by  $\mathcal{P}$ . In other words the physical amplitude can be completely derived from the global  $T$ -matrix element  $\tilde{T}(\mathbf{k}'_\beta, \mathbf{k}_\alpha)$ .

**7. An illustrative example.** — We consider here a system of 5 fermions and assume, for the sake of simplicity, that there is only one bound state in each of the two, three and four-body systems. The corresponding self-energies are labelled  $E_2, E_3$  and  $E_4$  respectively. We are interested in a collision where a projectile of two nucleons drops one nucleon on the three-nucleon target. The various channels of interest are, in an obvious notation

$\alpha$	(2) + (3)	10	
$\beta$	(1) + (4)	5	
$\gamma$	(1) + (1) + (3)	10	(7.1)
$\delta$	(1) + (2) + (2)	15	
$\eta$	(1) + (1) + (1) + (2)	10	
$\omega$	(1) + (1) + (1) + (1) + (1)	1	

where we have also shown the number of non equivalent partitions for each channel.

Because of the constraint  $\sum_i \mathbf{k}_i = \sum_i \mathbf{k}'_i = 0$ , the global  $T$ -matrix element  $\tilde{T}(\mathbf{k}', \mathbf{k})$  is a function of 50 independent variables, including  $W$ . We define

$$\mathbf{k}_\alpha = \mathbf{k}_1 + \mathbf{k}_2 = -(\mathbf{k}_3 + \mathbf{k}_4 + \mathbf{k}_5),$$

and retain only  $\mathbf{k}_1$  to  $\mathbf{k}_4$  as independent variables. In the same way we retain only  $\mathbf{k}'_1$  to  $\mathbf{k}'_4$  and define  $\mathbf{k}'_\beta = \mathbf{k}'_1$ . We then freeze  $W$ , and the combinations

$$\begin{aligned} \kappa_1 &= \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2), & \kappa_2 &= \frac{1}{2}(\mathbf{k}_3 - \mathbf{k}_4), \\ \kappa_3 &= -\frac{2}{3}(\mathbf{k}_1 + \mathbf{k}_2) - (\mathbf{k}_3 + \mathbf{k}_4), \\ \kappa'_1 &= \frac{1}{2}(\mathbf{k}'_3 - \mathbf{k}'_4), & \kappa'_2 &= \mathbf{k}'_2 + \frac{1}{2}(\mathbf{k}'_1 + \mathbf{k}'_3 + \mathbf{k}'_4), \\ \kappa'_3 &= \frac{1}{2} \mathbf{k}'_1 + \mathbf{k}'_3 + \mathbf{k}'_4. \end{aligned} \tag{7.2}$$

The on-shell conditions read

$$\frac{\hbar^2}{2\mu_\alpha} k_\alpha^2 = W - E_2 - E_3, \quad \mathbf{k}_\alpha = \mathbf{k}_1 + \mathbf{k}_2,$$

and

$$\frac{\hbar^2}{2\mu_\beta} k'^2_\beta = W - E_4, \quad \mathbf{k}'_\beta = \mathbf{k}'_1. \tag{7.3}$$

This defines in the 48-dimensional space  $\mathbf{k}_1 \dots \mathbf{k}_4, \mathbf{k}'_1 \dots \mathbf{k}'_4$  a locus of dimension 44. Let  $\mu$  be the nucleon mass. Any additional on-shell condition, for a break-up channel  $\gamma$  for instance in the partition 1 + 2 + (345),

$$\frac{2\hbar^2}{3\mu} \left( \frac{4\mathbf{k}'_2 + \mathbf{k}'_1}{4} \right)^2 + \frac{5\hbar^2}{8\mu} k'^2_1 = W - E_3, \tag{7.4}$$

reduces in general the locus given by eqs. (7.3) to a smaller locus of dimension at most 42. For, obviously, eq. (7.4) is not a consequence of eqs. (7.3). It is therefore always possible to choose  $\kappa_1 \dots \kappa'_3$  so that the resulting point in the locus defined by eqs. (7.3) lies away from that defined by eq. (7.4). Because only scalars are involved the orientations  $\hat{k}_\alpha, \hat{k}'_\beta$  are completely free.

Any additional choice of channel and partition generates a condition analogous to eq. (7.4). The intersection of all those loci with the locus defined by eqs. (7.3) remains of dimension 42, for the number of loci is finite, as shown by the table (7.1). It is indeed smaller than  $10 + 15 + \dots + 1 = 36$ .

This proves that the choice of momenta which induce on-shell properties for two channels only and *exclude* on-shell properties for any partition of any other channel is bound to succeed.

Returning now to the problem of partitions in the only two channels which remain on-shell, it is clear for instance that if particles 1 and 2 are permuted in the channel  $\beta$ , the corresponding  $\bar{\mathbf{k}}'_\beta$  becomes  $\bar{\mathbf{k}}'_2$ . The on-shell condition

$$\frac{\hbar^2}{2\mu_\beta} \bar{\mathbf{k}}'^2_\beta = W - E_4, \quad (7.5)$$

can then trivially be made incompatible with eqs. (7.3) by a suitable choice of the  $\mathbf{k}'_1, \mathbf{k}'_2, \mathbf{k}'_3$ .

Although very tedious in practice, this procedure shows that the proper identification of the singularities of the Möller operators  $\Omega$  is feasible.

**8. A variational principle.** — We want now to estimate  $\tilde{T}(\mathbf{k}', \mathbf{k})$ . We first consider completely off-shell conditions. Namely we select i)  $W$  complex and ii) all momenta  $\mathbf{k}, \mathbf{k}'$  so that no equation like eqs. (7.3) be satisfied, for any channel and partition.

Furthermore we take great care that  $\tilde{T}$  should contain no contribution from disconnected graphs. For that purpose,  $\mathbf{k}$  and  $\mathbf{k}'$  are chosen so that any  $\mathbf{k}_i$  is never equal to any  $\mathbf{k}'_j$ , nor any sum  $(\mathbf{k}_i + \mathbf{k}_k)$  to any sum  $(\mathbf{k}'_j + \mathbf{k}'_l)$  and so on. This is again always possible, and compatible with off-shell conditions.

In order to evaluate  $\tilde{T}(\mathbf{k}', \mathbf{k})$  for complex values of  $\mathbf{k}', \mathbf{k}$  one may think first of evaluations for real values of these vectors, followed by an analytic continuation. It is interesting to point out that, when  $W$  is complex, all the real values of  $\mathbf{k}$ , and  $\mathbf{k}'$  are off-shell since the conditions such as eqs. (7.3) to (7.5) are polynomials with real coefficients except  $W$ .

For real values of  $\mathbf{k}$  we thus consider the wave-packet

$$|\mathbf{k}\Delta\rangle = \lambda(\Delta) \int d\mathbf{p} \Gamma\left(\frac{\mathbf{p} - \mathbf{k}}{\Delta}\right) \mathcal{A}|\mathbf{p}\rangle, \quad (8.1)$$

where  $|\mathbf{p}\rangle \equiv |\mathbf{p}_1 \dots \mathbf{p}_N\rangle$  is a ket like that defined by eq. (2.5) with real momenta  $\mathbf{p}$  and the weight function  $\Gamma$ , of *finite* extension  $\Delta$ , is suitably normalized by the proper coefficient  $\lambda(\Delta)$ . It is clear that the wave-packet  $|\mathbf{k}\Delta\rangle$  will induce an average of purely off-shell situations around  $\mathbf{k}$ . The *finite* extension  $\Delta$  is chosen to prevent any dangerous, unconnected contribution to creep in through the wave-packets.

The matrix element of the global  $T$ -operator

$$\tilde{T}(\mathbf{k}', \mathbf{k}, \Delta) = \langle \mathbf{k}'\Delta | [V + VG(W)V] | \mathbf{k}\Delta \rangle \quad (8.2)$$

is then an average of purely off-shell matrix elements. The global off-shell  $T$ -operator  $T(W)$ , with  $W$  complex, is *a priori* regular for all off-shell momenta, in a neighbourhood of  $(\mathbf{k}', \mathbf{k})$ . The off-shell matrix element between plane waves is then the limit

$$\tilde{T}(\mathbf{k}', \mathbf{k}) = \lim_{\Delta \rightarrow 0} \tilde{T}(\mathbf{k}', \mathbf{k}, \Delta) \quad (8.3)$$

obtained when the packets  $\Gamma$  are shrunk to zero width.

The technical advantage of the matrix element  $\tilde{T}(\mathbf{k}', \mathbf{k}, \Delta)$  is that the bra and ket are square integrable. The functional

$$F(\chi', \chi) \equiv \langle \chi' | (W - K) | \mathbf{k}\Delta \rangle + \langle \mathbf{k}'\Delta | (W - K) | \chi \rangle - \langle \chi' | (W - H) | \chi \rangle \quad (8.4)$$

is then in principle easy to calculate for any square integrable trial functions  $\chi, \chi'$ . The stationarity conditions of  $F$  with respect to  $\chi$  and  $\chi'$  then read

$$|\chi\rangle = (W - H)^{-1} (W - K) | \mathbf{k}\Delta \rangle = [1 + (W - H)^{-1} V] | \mathbf{k}\Delta \rangle, \quad (8.5)$$

$$\langle \chi' | = \langle \mathbf{k}'\Delta | (W - K) (W - H)^{-1} = \langle \mathbf{k}'\Delta | [1 + V(W - H)^{-1}].$$

As long as  $W$  is complex they guarantee that  $\chi$  and  $\chi'$  are square integrable.

The stationary value of  $F$  is thus

$$F^s(\mathbf{k}', \mathbf{k}, \Delta) = \langle \mathbf{k}'\Delta | (W - K) (W - H)^{-1} \times (W - K) | \mathbf{k}\Delta \rangle = \langle \mathbf{k}'\Delta | (W - H + V) \times [1 + (W - H)^{-1} V] | \mathbf{k}\Delta \rangle = \tilde{T}(\mathbf{k}', \mathbf{k}, \Delta) + \langle \mathbf{k}'\Delta | (W - K) | \mathbf{k}\Delta \rangle. \quad (8.6)$$

In the limit  $\Delta \rightarrow 0$  the matrix element

$$\langle \mathbf{k}'\Delta | (W - K) | \mathbf{k}\Delta \rangle$$

vanishes as soon as  $\mathbf{k}'$  and  $\mathbf{k}$  are not strictly identical, which is indeed the case. According to eq. (8.3) this limit of  $F^s$  gives therefore the completely off-shell element  $\tilde{T}(\mathbf{k}', \mathbf{k})$  between real plane waves.

It can be concluded that the variational principle based on  $F$ , eq. (8.4), followed by the limit, eq. (8.3), gives a possible calculation of the off-shell elements  $\tilde{T}$  if a sufficiently large class of trial functions  $\chi$  and  $\chi'$  can be used.

Alternately one may use a variational principle based on the functional

$$F'(\chi', \chi) = \langle \mathbf{k}'\Delta | V | \chi \rangle + \langle \chi' | \mathbf{k}\Delta \rangle - \langle \chi' | (1 - G_0 V) | \chi \rangle \quad (8.7)$$

which is obviously related to that of Lemmer and Hufner [13]. But this functional  $F'$  is not symmetric and will not be discussed here.

The last step is the analytic continuation of the off-shell elements  $\tilde{T}(\mathbf{k}', \mathbf{k})$  from real to complex off-shell values of  $\mathbf{k}, \mathbf{k}'$ . Let  $\mathbf{k}, \mathbf{k}'$  be such complex off-shell values. As later  $\mathbf{k}$  and  $\mathbf{k}'$  will be made on-shell, it is interesting to choose  $\mathbf{k}$  and  $\mathbf{k}'$  *between* the domain of real momenta and the smooth hypersurfaces defined by the equations of energy conservation.

Indeed the complex domain of  $\mathbf{k}, \mathbf{k}'$  makes a space

of dimension  $12N - 12$ , the real domain of these vectors makes a subspace of dimension  $6N - 6$  and the quadratic loci defined by eqs. (7.3) to (7.5) for instance have no real points for  $W$  complex. There is thus always a path starting from the real domain, terminating on-shell and with all its intermediate points off-shell.

A folding operation with  $\mathbf{p}, \mathbf{p}'$  real and  $\mathbf{k}, \mathbf{k}'$  complex on such a path

$$\tilde{T}(\mathbf{k}', \mathbf{k}, \Delta) = |\lambda(\Delta)|^2 \times \int d\mathbf{p} d\mathbf{p}' \Gamma\left(\frac{\mathbf{k} - \mathbf{p}}{\Delta}\right) \Gamma\left(\frac{\mathbf{k}' - \mathbf{p}'}{\Delta}\right) \tilde{T}(\mathbf{p}', \mathbf{p}) \quad (8.8)$$

followed by the suitable limit  $\Delta \rightarrow 0$  provides then  $\tilde{T}(\mathbf{k}', \mathbf{k})$ . We point out here that all the paths starting from  $\mathbf{p}, \mathbf{p}'$  and arriving at  $\mathbf{k}, \mathbf{k}'$  remain in the regularity domain of off-shell matrix elements as  $\mathbf{p}$  and  $\mathbf{p}'$  are integrated upon. Here  $\Gamma$  can be a truncated Gaussian, the analytic continuation of which is trivial.

A short cut combining the use of wave-packets and analytic continuation consists in setting  $\mathbf{k}$  and  $\mathbf{k}'$  off-shell and complex directly in eq. (8.1) and carry the steps up to eq. (8.6) or (8.7). For obvious reasons of mathematical caution we have first described in this section separately the wave-packet limit and the analytic continuation. It is clear, however, that one may expect analyticity properties of the fully connected part of  $\tilde{T}(\mathbf{k}', \mathbf{k})$  in the neighbourhood of an *off-shell* and *necessarily connected* configuration of momenta  $(\mathbf{k}', \mathbf{k})$  if the interactions  $V_{ij}$  are sufficiently short-ranged.

**9. Discussion and conclusion.** — Once the global  $T$ -matrix operator has been defined, there are three major steps in the calculations derived from the present theory. The first consists in the calculation of off-shell matrix elements for complex energy and momenta. This is provided by a variational principle between wave-packets and normalized trial functions, an *a priori* safe procedure. It should be noted that the variational principle suggested here is different from the one formulated for the channel transition amplitudes [14]. The accuracy of the variational calculation, however, obviously depends on the richness of the space of trial functions like in all variational approaches. The limit from wave-packets to plane waves is taken after the variational calculation, which is the correct approach.

The second step consists in the selection of specific channel amplitudes by a limit to on-shell, still in the complex domain. Although the identification of the nature of the singularities which occur in this on-shell limit is difficult, we have gone a long way towards showing that the other channels can be prevented from contaminating the residue. This is obtained by proper selections of the Jacobi momenta which do not go on-shell. While the complete investigation of

all possible channels contaminations is *a priori* tedious, it has been proved that it is in principle possible. Furthermore the equations of on-shell limit can be written in terms of the single particle momenta, thus making the theory perfectly symmetric. We have proved that the identification of channels is easily compatible with the Pauli principle. The Galilean invariance of the procedure is also explicit.

The last step is the limit for a real energy of the residue obtained by the second step. As long as the energy is complex the resolvent is that regular operator which converts normalizable states into normalizable states. As  $+i\epsilon \rightarrow 0$  the limit of the totally on-shell amplitude extracted as a residue is then identified with the usual physical amplitude  $T_{\beta\alpha}^{(+)}$  with outgoing boundary conditions. A more detailed analysis of this limit is necessary in order to confirm the identification with the physical outgoing amplitude. It is already gratifying at this stage of the theory to have a well defined, unique limit prescription.

The main problem in this theory is the practical calculation of the matrix elements of  $T$ . While this calculation can be related to more traditional theories of coupled channels and may be guided by a variational principle, some more practical investigation is clearly needed. The connected kernel methods [15] developed by various authors would very likely improve our understanding of numerical algorithms. It can be noted that Slater determinants can be used as trial functions in the variational principle. This may relate the theory with Hartree-Fock-like approximations.

While the theory is still formal, its main interest lies in its perfect symmetry. Only symmetric operators such as the total potential or kinetic energies appear. Specific channels are *recognized*, rather than introduced *a priori*. The recognition of the channels is accomplished through a prior calculation of the cluster binding energies,  $E_m^\alpha, E_n^\beta$ . This demands only diagonalization of the full Hamiltonian for smaller numbers of particles and for a few of their bound states. In particular, the use of the global  $T$ -operator demands that the channel states appear directly from the analytic properties of the total Green's function. This stresses the importances of consistent approximations in the evaluation of transition amplitudes.

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