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The Unitarity of the S Matrix for Multichannel Scattering

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Abstract. The usual proofs for the unitarity of the S matrix are based on the assumption that the wave functions in different channels are orthogonal to each other. This is not the case in rearrangement collisions where the colliding particles and the collision products are composite fragments (overlapping channels).

A correct proof for the usual unitarity property of the S matrix is given for the case of overlapping channels. The proof is greatly facilitated by a systematic use of the spectral representation for a complete system of commuting observables.

Each channel defines as a consequence of the asymptotic condition a pair of wave operators. These are partial isometries with orthogonal ranges for different channels. This orthogonality property, which was proved in an earlier paper, is the essential property which implies unitarity for the S matrix in the usual sense. Unitarity is then shown to be a direct consequence of the asymptotic condition and nothing more.

I. Introduction

The unitarity of the S matrix for general reaction and scattering processes is generally postulated as a basic property in all treatments of such processes. It would therefore be of the greatest interest to know the physical foundation for this property. In the case of simple scattering systems (one channel only) the unitarity of the S matrix can indeed be thus related to the asymptotic condition which expresses the fundamental property of any scattering system that the interaction between the scattered particles is described by an energy operator which differs from the kinetic energy of the particles only in a finite region of space. Thus for one-channel systems one has a perfectly satisfactory explanation, in physical terms, for the unitarity property of the S matrix.

One has tried, by an obvious adaptation of this reasoning to extend this explanation to the case of many-channel scattering. However all of these reasonings are either based on the assumption that the wave functions in different channels are orthogonal to each other [1][1]) or they use reasonings which are mathematically insufficient and have therefore only an exploratory significance [2].

The difficulty has been noted by many people and has been discussed in numerous publications, of which we cite a representative selection [3–7].

Let us examine in this introduction a commonly used "proof" for the unitarity of the S matrix, such as it is found for instance in Ref. [1].

[1]) Numbers in brackets refer to References, page 337.

Consider the situation sketched schematically in Figure 1.

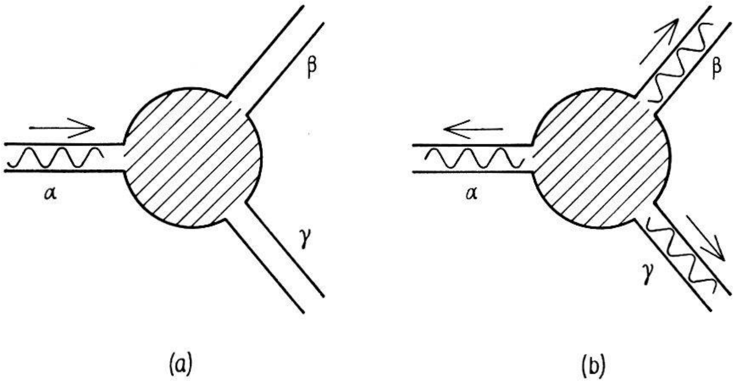

Figure 1

Schematic representation of a three channel scattering process.
a) Situation before scattering: incident wave in channel α approaches scattering region (shaded area).
b) Situation after scattering: outgoing waves in the three channels escape from scattering region.

Initially, the system is supposed to be in channel α. After the reaction has occurred the system is distributed over all the open channels and the probability amplitude in channel β is $S_{\alpha\beta}$. Thus the probability of finding the system after the collision in channel β (when it was in channel α *before* the collision) is therefore given by $| S_{\alpha\beta} |^2$. Using now the constancy of the norm of the wave function Ψ one concludes that

$$(\Psi, \Psi) = 1 = \sum_\beta | S_{\alpha\beta} |^2 . \tag{1.1}$$

A slight generalization of this same argument, using the constancy of the scalar product of any pair of wave functions leads to

$$\sum_\beta S^*_{\alpha\beta} \, S_{\gamma\beta} = \delta_{\alpha\gamma} . \tag{1.2}$$

If this relation is written as an operator relation, interpreting $S_{\alpha\beta}$ as the matrix element of an operator S, it becomes

$$S^* S = I , \tag{1.3}$$

which is one half of the unitarity relation. The other half

$$S \, S^* = I \tag*{(1.3)*}$$

is usually assumed to be also true, although it is in fact a new and independent relation.

The validity of this "proof" for the relation (1.3) depends in an essential way on the assumption that the different channels are orthogonal to one another. Indeed, if we have a superposition of normalized wave functions Ψ_β in different channels of the form $\Psi = \sum_\beta S_{\alpha\beta} \Psi_\beta$, then the norm of this function is given by

$$(\Psi, \Psi) = \sum_{\beta'\beta''} S^*_{\alpha\beta'} \, S_{\alpha\beta''} \, (\Psi_{\beta'}, \Psi_{\beta''}) . \tag{1.4}$$

This is only equal to the right-hand side of (1.1) if $(\Psi_{\beta'}, \Psi_{\beta''}) = \delta_{\beta'\beta''}$.

It is easy to see with simple examples that this assumed orthogonality is not always satisfied. Let us for instance examine the scattering of a deuteron on a fixed centre of force. If the incident energy is larger than the binding energy of the deuteron then there are two open channels for the final states, namely the deuteron, or the free proton-neutron (cf. Figure 2).

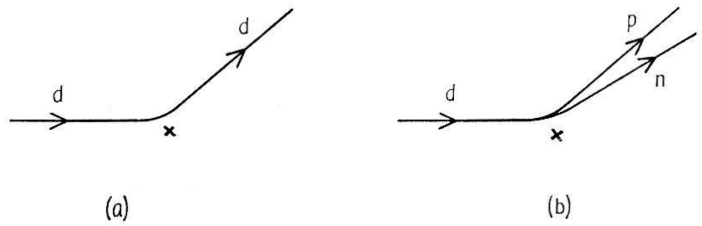

Figure 2

An example of a two-channel reaction with non-orthogonal channels: the final states of reaction (a) are linear combinations of the final states of reaction (b).

Since the deuteron is a composite particle, containing as its constituents a proton and a neutron, we cannot assume these channels to be orthogonal. Indeed, in the elementary theory of the deuteron, one calculates precisely the matrix element of the deuteron in an orthogonal proton-neutron system. This matrix element is the wave-function of the deuteron.

On the other hand there are cases where the assumed orthogonality may be satisfied, for instance always then when transitions from one system of elementary particles to another system of such particles are considered. The problem occurs only for transitions involving composite particles. Such transitions are often more explicity denoted as *rearrangement collisions*.

The question then reduces to this: is the S matrix unitary also for rearrangement collisions?

It was pointed out by Ekstein [3] that in general there does not exist a linear operator the matrix elements of which are the S matrix elements for a multichannel system. Subsequently, Jauch [8] has shown that for simple scattering systems one can define two different unitary operators which can be related to the S matrix elements in a simple way. Only one of these operators can be generalized to the multichannel case and again the S matrix elements are related easily to this operator. It will be seen in the following that the consideration of this operator will be very useful in the proof of the unitarity property of the S matrix for rearrangement collisions.

It should be remarked that the distinction whether certain particles are composite or elementary is notoriously difficult to answer, be it from the experimental or theoretical point of view. This difficulty has incited some to declare it as meaningless, or at least irrelevant, and to replace it by a self-consistent formalism ("bootstrap" calculations) where each particle is in a sense elementary and composite at the same time.

We point out here that if the S matrix for rearrangement collisions were not exactly orthogonal, but satisfied instead a relation such as (1.4), this procedure would be doomed to failure from the start, since the relation (1.4) would permit us to make a clear distinction between elementary and composite particles.

The result of this paper will thus be that unitarity in the usual form is generally valid, even for overlapping channels, and it is not possible to distinguish elementary from composite particles by a consideration of the S matrix alone.

In the course of the proof we have made extensive use of an important mathematical tool, the spectral representation, established in a previous publication [9]. This tool enables us to dispense entirely with the expansion in non-normalizable eigenfunctions of the energy operator. This expansion procedure is almost exclusively used by physicists today and it is a source of major mathematical difficulties. Because there are not sufficiently strong theorems available concerning such expansions, most of the results obtained so far with such methods are open to questions.

For the convenience of the reader, not familiar with Ref. [9], we shall briefly recapitulate in Section 2, in elementary terms and without proofs, the results obtained therein. They are slightly generalized and adapted to the needs of the problem on hand. In Section 3 we give then with the aid of this tool, the proof of the unitarity condition for the multichannel scattering matrix.

II. The Spectral Representation for a Complete System of Commuting Observables (C.S.C.O.)

In this Section we shall review some of the basic notions of mathematical nature needed for the subsequent part of this paper. All results will be stated without proof. The necessary proofs for establishing the spectral representation in sufficient generality were given in Ref. [9]. Here we merely state some selected results from this paper for convenience, as well as some easy corollaries and generalizations not mentioned in this paper.

Let $A_1, A_2, \ldots, A_n$ be a C.S.C.O. They are a set of n self-adjoint operators in a Hilbert space $\mathcal{H}$, which commute pairwise and generate a maximal Abelian algebra of operators in $\mathcal{H}$. We shall assume that the spectrum Λ_r of the operator A_r is a (closed) segment of the real line. There are thus no discrete eigenvalues and no eigenvectors in $\mathcal{H}$ for A_r. (This is the situation encountered in scattering theory.) We denote by $\Lambda = \Lambda_1 \times \Lambda_2 \times \cdots \times \Lambda_n$ the Cartesian product of the spectra. An element $\lambda \in \Lambda$ is thus the n-tupel of numbers $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_n)$, with $\lambda_r \in \Lambda_r$.

The theorem on the spectral representation affirms the existence of a uniquely determined measure class $[\varrho]$ on Λ (which will contain Lebesgue measure in our applications) and an isomorphism between the abstract Hilbert space $\mathcal{H}$ and the function space $L^2_\varrho(\Lambda)$ of square integrable functions over Λ which associates with each element $x \in \mathcal{H}$ a function $f(\lambda) \in L^2_\varrho(\Lambda)$.

In order to facilitate the statement of the properties of this isomorphism we introduce the following slight generalization of Dirac's bra-ket notation.

The function $f(\lambda)$, image of $x \in \mathcal{H}$ in the above-mentioned isomorphism, will be denoted by $\langle \lambda \mid x)$. The complex conjugate of this function will be denoted by $(x \mid \lambda\rangle \equiv \langle \lambda \mid x)^*$. The isomorphism is then expressed by the following relations

$$\langle \lambda \mid x + y) = \langle \lambda \mid x) + \langle \lambda \mid y) \text{ for all } x, y \in \mathcal{H}$$

$$\langle \lambda \mid \theta\, x) = \theta \langle \lambda \mid x) \text{ for all complex } \theta \tag{2.1}$$

$$(x, y) = \int_\Lambda (x \mid \lambda \rangle \langle \lambda \mid y)\, d\varrho(\lambda)\,. \tag{2.2}$$

The measure $d\varrho(\lambda)$ in this last equation will be the Lebesgue measure on the Cartesian product space for all applications of this paper and will be denoted simply by $d\lambda$ in the following.

The usefulness of this isomorphism is due to the fact that it can be so constructed that the operators A_r ($r = 1, \ldots, n$) are multiplication operators:

$$\langle \lambda \mid A_r x) = \lambda_r \langle \lambda \mid x) \tag{2.3}$$

provided that they satisfy a condition stated in Ref. [9] which characterizes them as "independent".

If $B = u\,(A_1 \ldots A_n)$ is a function of the operators A_r then we have

$$\langle \lambda \mid B\,x) = u(\lambda_1 \ldots, \lambda_n) \langle \lambda \mid x)\,. \tag{2.4}$$

Operators of this kind are said to be "diagonalized" in the spectral representation. They are then multiplication operators in $L^2(\Lambda)$.

An important class of more general operators are those which can be represented as integral operators in $L^2(\Lambda)$. For such an operator T we may thus write

$$\langle \lambda \mid T\,x) = \int \langle \lambda \mid T \mid \lambda' \rangle \langle \lambda' \mid x)\, d\lambda'\,. \tag{2.5}$$

Here $\langle \lambda \mid T \mid \lambda' \rangle$ is the kernel of the integral operator. We shall also call it the representation of the operator T in the spectral representation. However not all operators T are of this kind. An equation such as (2.5) is often interpreted in the literature as a symbolic equation for a distribution. Since this extended symbolic meaning of the Equation (2.5) can cause mathematical difficulties we shall avoid it in this paper and restrict the use of Equation (2.5) to bona fide integral operators.

Of special interest in the following will be operators which commute with some function of the A_r. Let T be such an operator and $H = H\,(A_1 \ldots A_n)$ the function of the A_r with which T commutes. We can then always choose (in many ways) a new set of commuting operators, containing H as a member, and such that they are again a new C.S.C.O. We change the notation here and designate from now on this system with $H, A_1, \ldots, A_n$. The Cartesian product of the spectra Λ_r of A_r will be denoted as before by $\Lambda = \Lambda_1 \times \Lambda_2 \times \ldots \times \Lambda_n$, and a general point of Λ will be denoted by λ.

We designate with E a point in the spectrum of H which we assume also to be continuous. The isomorphism of the spectral representation takes then the form $x \to \langle E\,\lambda \mid x)$.

An operator T which commutes with H is diagonal with respect to the variable E so that it may be written in the form

$$\langle E\,\lambda \mid T\,x) = \int \langle \lambda \mid T(E) \mid \lambda' \rangle \langle E\,\lambda' \mid x)\, d\lambda'\,. \tag{2.6}$$

In the subsequent applications the operator H will be an energy operator and the operator T of (2.6) is then said to be an operator "on the energy shell".

For every fixed value of E and every $x \in \mathcal{H}$ the functions $\langle E\,\lambda \mid x)$ are square integrable over the variables λ. They are thus themselves a Hilbert space which we denote by $\mathcal{H}(E)$. The function $\langle E\,\lambda \mid x)$ is then the spectral representation of a vector $x(E) \in \mathcal{H}(E)$. Thus we have explicitly constructed a "direct integral" of Hilbert spaces $x = \{x(E)\}$ with $\| x \|^2 = \int \| x(E) \|^2 \varrho(E)\, dE$, where $\varrho(E)$ is some density function proportional to the volume of the energy shell.

In this representation the operator T which commutes with H may also be written as a direct integral by setting

$$T\{x(E)\} = \{T(E)\, x\,(E)\}\,. \tag{2.7}$$

This is the abstract version of (2.6), but it is correct even for the more general case that $T(E)$ is not an integral operator on the energy shell.

In the following applications we also need the formulae for a change of the spectral representation. These are the obvious generalizations of the formulae for the change of a coordinate system.

We begin with the simplest special case which suffices as a point of departure for the more general formulae needed in multichannel scattering theory.

Let us assume first that there exist two energy operators H_0 and H which are unitarily equivalent so that their spectra are identical. There exists then a unitary operator Ω which has the intertwining property

$$H\,\Omega = \Omega\,H_0\,. \tag{2.8}$$

This is the situation for the simple scattering systems without bound states, which we examine here first for the purpose of introducing the concept of the transformation of the spectral representation. The generalization to the multichannel situation will the be easy and will be made later on.

For this special case the operator Ω is unitary

$$\Omega^*\,\Omega = I = \Omega\,\Omega^*\,, \tag{2.9}$$

so that $\Omega^* = \Omega^{-1}$.

The operator Ω is not unique if the spectra of H and H_0 are degenerate. It can thus be subjected to additional restrictions which in scattering theory are dictated by the physical situation of a scattering process. For the moment we shall not need to specify these conditions.

Just as in finite-dimensional spaces, we can, here too, interpret the operator Ω in two ways. We can consider it as a transformation of the vector space $\mathcal{H}$ which assigns to any $x \in \mathcal{H}$ the transformed $\Omega\,x$. We can also interpret Ω as a change of the reference system in a particular representation of the space. Thus Ω will induce a change of the spectral representation.

Let us denote by ${}_0\langle E\,\lambda \mid x)$ the spectral representation of the vector x with respect to H_0 and a certain number of additional operators $A_1, \dots, A_n$ needed to obtain a complete system of observables. We define then a new spectral representation $\langle E\,\lambda \mid x)$ by setting

$$\langle\, E\,\lambda \mid x) \equiv {}_0\langle\, E\,\lambda \mid \Omega^*\,x)\,. \tag*{$(2.10)_0$}$$

We claim that $\langle E\,\lambda \mid x)$ is the spectral representation of x with respect to H. In fact

$$\langle\, E\lambda \mid H\,x) = {}_0\langle\, E\lambda \mid \Omega^*\,H\,x) = {}_0\langle\, E\lambda \mid H_0\Omega^*\,x) = E\,{}_0\langle\, E\lambda \mid \Omega^*\,x) = E\,\langle\, E\lambda \mid x)\,. \tag{2.11}$$

Substituting $\Omega\,x$ for x we obtain the reverse relation to $(2.10)_0$

$${}_0\langle E\,\lambda \mid x) = \langle E\,\lambda \mid \Omega\,x)\,. \tag*{$(2.10)_1$}$$

The representation which we have constructed here is the spectral representation with respect to the new C.S.C.O. $\{H, \Omega\,A_r\,\Omega^*\}$ $(r = 1, \dots, n)$, in fact

$$\langle\, E\,\lambda \mid \Omega\,A_r\,\Omega^*\,x) = {}_0\langle\, E\,\lambda \mid A_r\,\Omega^*\,x) = \lambda_r\,{}_0\langle\, E\,\lambda \mid \Omega^*\,x) = \lambda_r\,\langle\, E\,\lambda \mid x)\,.$$

We now proceed to generalize first to the case where the intertwining operator Ω is no longer unitary but only an isometry. Instead of the relation (2.9) we have then

$$\Omega^* \Omega = I\,, \quad \Omega \Omega^* = F < I \tag{2.12}$$

where F is the projection operator onto the range of Ω. Equation (2.11) is then still valid for all x in the range of Ω, that is all x which satisfy $F x = x$. The equation is valid for all $x \in \mathcal{H}$ if we replace in (2.11) the operator H by $F H = H F = F H F$. It is thus the spectral representation of the operator $F H F$.

Let us now examine the transformation of operators under change of the spectral representation. Let T be an operator which commutes with H_0 and assume further that in the spectral representation ${}_0\langle E\,\lambda \mid x)$ it is a bona fide integral operator, so that we may write

$${}_0\langle E\,\lambda \mid T\,x) = \int {}_0\langle \lambda \mid T(E) \mid \lambda' \rangle_0\, {}_0\langle E\,\lambda' \mid x)\, d\lambda'\,. \tag{2.13}$$

It follows then from

$$\begin{aligned}\langle E\,\lambda \mid \Omega\,T\,\Omega^*\,x) &= {}_0\langle E\,\lambda \mid T\,\Omega^*\,x) = \int {}_0\langle \lambda \mid T(E) \mid \lambda' \rangle_0\, {}_0\langle E\,\lambda' \mid \Omega^*\,x)\, d\lambda' \\ &= \int {}_0\langle \lambda \mid T(E) \mid \lambda' \rangle_0\, \langle E\,\lambda' \mid x)\, d\lambda'\end{aligned}$$

that $\Omega\,T\,\Omega^*$ is an integral operator in the H-representation with the kernel

$$\langle E\,\lambda \mid \Omega\,T\,\Omega^* \mid E\,\lambda' \rangle = {}_0\langle \lambda \mid T(E) \mid \lambda' \rangle_0\,.$$

Thus the operator $\Omega\,T\,\Omega^*$ is on the energy-shell in the new representation which is conform to the fact that $\Omega\,T\,\Omega^*$ commutes with H, and we may use the notation

$$\langle E\,\lambda \mid \Omega\,T\,\Omega^* \mid E\,\lambda' \rangle = \langle \lambda \mid \Omega\,T\,\Omega^*(E) \mid \lambda' \rangle = {}_0\langle \lambda \mid T(E) \mid \lambda' \rangle_0\,. \tag{2.14}$$

For the treatment of multichannel scattering problems we need to generalize these results still further. We must deal with situations where we have not just one energy operator H_0 but a whole sequence of "channel operators" H_α ($\alpha = 1, 2, \ldots$). The channel index α distinguishes the different channels. The domain of α may be finite or infinite, but it is always countable [8]. The channel operators H_α are the energy operators for the free particles in channel α.

If the system is a multichannel scattering system then there exist sequences of intertwining operators $\Omega^{(\alpha)}$ ($\alpha = 1, 2, \ldots$) with the properties

$$H\,\Omega^{(\alpha)} = \Omega^{(\alpha)}\,H_\alpha \tag{2.15}$$

and

$$\Omega^{(\alpha)*}\,\Omega^{(\alpha)} = E_\alpha$$

$$\Omega^{(\alpha)}\,\Omega^{(\alpha)*} = F_\alpha\,. \tag{2.16}$$

The projection operators E_α and F_α are in general different from the unit operator. Hence the $\Omega^{(\alpha)}$ are in general no longer unitary, they are only *partial isometries*.

Corresponding to this notion of partial isometries we may introduce the notion of the *partial spectral representation*. While the ordinary spectral representation so far considered furnishes an isomorphic mapping of the entire Hilbert space $\mathcal{H}$ onto an L^2 space of functions, the partial spectral representation maps only a proper subspace

$M \subset \mathcal{H}$ onto such a function space. In order to formulate this situation properly we revert for a moment to the one-channel formalism, the generalization to the multichannel being then obtained by adding in the subsequent formulae a channel index at the proper place.

We assume then that we are given a free evolution operator H_0 together with a C.S.C.O. $A_1, \ldots, A_n$, all of which leave a proper subspace $M \subset \mathcal{H}$ invariant. This means that the projection operator E with range M commutes with H_0 and all A_r. We say M (or E) *reduces* the operators H_0 and A_r. Instead of the operators H_0 and A_r, we may then consider their reductions to the subspace M, that is the operators $H_0 E = E H_0$, and $A_r E = E A_r$. These operators, if they are complete, generate a maximal Abelian algebra in M. The theorem of the spectral representation can now be taken over word for word by substituting the subspace M for the space $\mathcal{H}$ in the previous formulation.

This leads to the following results:

There exists a uniquely defined measure class $[\varrho]$ on the product space of the spectra of $H_0 E$ and $A_r E$ and an isomorphism of M to the Hilbert space L^2_ϱ of functions over the spectra of these operators. If we denote by ${}_0\langle E\,\lambda \mid x)$ the function in L^2_ϱ which corresponds to the vector $x \in M$ then we have for this function again the relations (2.1) and (2.2) of this section with the only change that M must be substituted for $\mathcal{H}$ in these formulae.

A change of the spectral representation can now be induced not only by a unitary operator as before; but more generally by a partial isometry. Indeed let Ω be a partial isometry with initial projection E and final projection F, so that $E = \Omega^* \Omega$ and $F = \Omega\, \Omega^*$. Let $M = E\,\mathcal{H}$ be the range of E and $N = F\,\mathcal{H}$ the range of F. The operator Ω furnishes then an isometric mapping of M onto N. Unlike the previous case, these two subspaces may be situated arbitrarily: M may have a common part with N or it may be entirely outside of N. In any case this partial isometry defines a transformed spectral representation which attributes to every $y \in N$, (that is every y of the form $y = \Omega\, x$, $x \in M$) the function

$$\langle E\,\lambda \mid \Omega\, x) \equiv {}_0\langle E\,\lambda \mid x)\,.$$

It is seen that this formula is identical with $(2.10)_0$. The only difference is that in the last formula the vectors x and $y = \Omega\, x$ range only over M and N respectively.

Returning now to the situation encountered in multichannel scattering we may for channel α assume the existence of a C.S.C.O. and thus define for each α a partial spectral representation ${}_\alpha\langle E\,\lambda_\alpha \mid x)$ for $x \in E_\alpha\,\mathcal{H}$, $(E_\alpha = \Omega^{(\alpha)*}\,\Omega^{(\alpha)})$. The partial isometry induces then a transformation of the spectral representation given by the formula

$$\langle E\,\lambda_\alpha \mid \Omega^{(\alpha)}\, x) \equiv {}_\alpha\langle E\,\lambda_\alpha \mid x)\,. \tag{2.10$_\alpha$}$$

It follows then from the intertwining property (2.15) that for each $y \in F_\alpha\,\mathcal{H}$, that is each y of the form $y = \Omega^{(\alpha)}\, x$; $x \in E_\alpha\,\mathcal{H}$ we have

$$\langle E\,\lambda_\alpha \mid H\, y) = E\,\langle E\,\lambda_\alpha \mid y) \tag{2.11$_\alpha$}$$

The transformed spectral representation $\langle E\,\lambda_\alpha \mid y)$ is thus diagonal for the operator $H\,F_\alpha$.

In the case of the multichannel scattering theory the projections F_α onto the range of $\Omega^{(\alpha)}$ are all orthogonal and their sum is the unit operator [8]:

$$F_\alpha F_\beta = \delta_{\alpha\beta} F_\beta \qquad \sum_\alpha F_\alpha = I . \tag{2.17}$$

In this case the isomorphism from the elements $y \in F_\alpha \mathcal{H}$ to the space $L^2(\Lambda^{(\alpha)})$ defined by (2.10) can be extended to an isomorphism of the entire space as follows: to every x we associate a *sequence* of functions $\langle E \lambda_\alpha \mid x)$ ($\alpha = 1, 2, \ldots$) in $L^2(\Lambda^{(\alpha)})$ by setting

$$\langle E \lambda_\alpha \mid x) \equiv \langle E \lambda_\alpha \mid F_\alpha x) = {}_\alpha\langle E \lambda_\alpha \mid \Omega^{(\alpha)*} x) . \tag{2.10}$$

Any linear operator can then be represented and studied in this extended spectral representation.

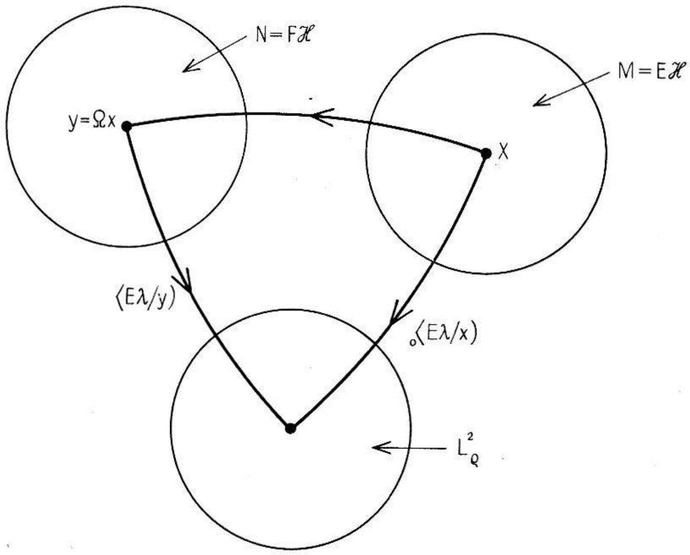

Figure 3

Illustration of the transformation of a partial spectral representation by a partial isometry.

In the following we shall be primarily interested in operators $T_{\alpha\beta}$ which have the intertwining property

$$H_\alpha T_{\alpha\beta} = T_{\alpha\beta} H_\beta . \tag{2.18}$$

This gives rise to the new notion of the *mixed spectral representation* of an operator. The operator $T_{\alpha\beta}$ maps a subspace $M_\beta = E_\beta \mathcal{H}$ into the subspace $M_\alpha = E_\alpha \mathcal{H}$. We shall consider the special case that the mapping is onto and is expressible as an integral operator such that

$${}_\alpha\langle E \lambda_\alpha \mid T_{\alpha\beta} x) = \int {}_\alpha\langle E \lambda_\alpha \mid T_{\alpha\beta} \mid E \lambda_\beta \rangle_\beta \, {}_\beta\langle E \lambda_\beta \mid x) \, d\lambda_\beta$$

valid for all $x \in M_\beta$. We have already implied with the notation that the operator $T_{\alpha\beta}$ is diagonal in the variable E as it follows from the intertwining property (2.18). In fact

$$\begin{aligned} {}_\alpha\langle E \lambda_\alpha \mid H_\alpha T_{\alpha\beta} \mid E' \lambda_\beta \rangle_\beta &= E \, {}_\alpha\langle E \lambda_\alpha \mid T_{\alpha\beta} \mid E' \lambda_\beta \rangle_\beta \\ &= {}_\alpha\langle E \lambda_\alpha \mid T_{\alpha\beta} H_\beta \mid E' \lambda_\beta \rangle_\beta = E' \, {}_\alpha\langle E \lambda_\alpha \mid T_{\alpha\beta} \mid E' \lambda_\beta \rangle_\beta \end{aligned}$$

therefore

$${}_{\alpha}\langle E\,\lambda_{\alpha} \mid T_{\alpha\beta} \mid E'\,\lambda_{\beta}\rangle_{\beta} = 0 \text{ for } E \neq E'$$

We shall use the notation

$${}_{\alpha}\langle \lambda_{\alpha} \mid T_{\alpha\beta}(E) \mid \lambda_{\beta}\rangle_{\beta} = {}_{\alpha}\langle E\,\lambda_{\alpha} \mid T_{\alpha\beta} \mid E\,\lambda_{\beta}\rangle_{\beta} \tag{2.19}$$

for the integral operator "on the energy shell". This representation of an intertwining operator is an example of a mixed spectral representation.

If $T_{\alpha\beta}$ has the intertwining property (2.18) then one verifies easily with the help of (2.15) that the operator $\Omega^{(\alpha)}\, T\, \Omega^{(\beta)*}$ commutes with H so that we may transform it to the spectral representation of H in analogy to the formula (2.14)

$${}_{\alpha}\langle \lambda_{\alpha} \mid T_{\alpha\beta}(E) \mid \lambda_{\beta}\rangle_{\beta} = \langle \lambda_{\alpha} \mid \Omega^{(\alpha)}\, T_{\alpha\beta}\, \Omega^{(\beta)*}(E) \mid \lambda_{\beta}\rangle\,. \tag{2.20}$$

In the following we shall also need the formula

$$\langle \lambda_{\alpha} \mid T_{\alpha\beta}\, F_{\gamma} \mid \lambda_{\beta}\rangle = \langle \lambda_{\alpha} \mid T_{\alpha\beta} \mid \lambda_{\beta}\rangle\, \delta_{\beta\gamma} \tag{2.21}$$

for any bona fide integral operator $T_{\alpha\beta}$ which maps the range of F_{β} onto the range of F_{α} and which commutes with H. Similarly, we may also affirm

$$\langle \lambda_{\alpha} \mid F_{\gamma}\, T_{\alpha\beta} \mid \lambda_{\beta}\rangle = \langle \lambda_{\alpha} \mid T_{\alpha\beta} \mid \lambda_{\beta}\rangle\, \delta_{\alpha\gamma}\,. \tag{2.22}$$

These formulae are easy consequences of the defining property of the spectral representations used here, and the orthogonality relations (2.17).

III. The Multichannel Scattering Matrix

For this section we shall need some of the results of a paper on the "Theory of the Scattering Operator II" [8], which will be briefly reviewed here.

A multichannel system is defined by a total energy operator H, together with some system of channel operators H_{α} which represent the kinetic energy of the free fragments in channel α.

The characteristic property of a scattering system is the *asymptotic condition* which affirms the existence of the limits

$$\Omega_{\pm}^{(\alpha)} = \lim_{t \to \mp\infty} V_t^*\, U_t^{(\alpha)} \tag{3.1}$$

where

$$V_t = e^{-iHt}\,, \quad U_t^{(\alpha)} = e^{-iH_{\alpha}t}\,.$$

The limit (3.1) is understood in the strong topology of the Hilbert space. It will in general only exist on some subspace $D_{\alpha} \subseteq \mathcal{H}$ with projection operator E_{α}. It can however be proved that the dimension of D_{α} is infinite [8]. The operators $\Omega_{\pm}^{(\alpha)}$ are partial isometries and E_{α} is defined by

$$\Omega_{\pm}^{(\alpha)*}\, \Omega_{\pm}^{(\alpha)} = E_{\alpha}\,. \tag{3.2}$$

The notation inaidentally implies that E_{α} is independent of the sign $\pm$. The ranges $R_{\pm}^{(\alpha)}$ of $\Omega_{\pm}^{(\alpha)}$ are closed linear subspaces and are also defined as the ranges of the projections

$$F_{\pm}^{(\alpha)} = \Omega_{\pm}^{(\alpha)}\, \Omega_{\pm}^{(\alpha)*}\,. \tag{3.3}$$

The matrix element for the scattering from channel α (with energy E and channel variables λ_α) into channel β (energy E and channel variables λ_β) is given by the matrix element of the operator $S_{\alpha\beta} \equiv \Omega_-^{(\alpha)*} \Omega_+^{(\beta)}$. This matrix element does not exist in the usual sense with respect to the energy variable since $S_{\alpha\beta}$ is an intertwining operator for the operators H_α and H_β (cf. Ref. [5])

$$H_\alpha S_{\alpha\beta} = S_{\alpha\beta} H_\beta . \tag{3.4}$$

The mixed representation of $S_{\alpha\beta}$ contains a "δ-function-like" kernel, and we can write a correct equation only if we use the diagonal spectral representation not for the operator $S_{\alpha\beta}$ but for $R_{\alpha\beta} = S_{\alpha\beta} - E_\alpha \delta_{\alpha\beta}$. For this operator we may in fact write (Equation (2.19))

$${}_\alpha\langle E\,\lambda_\alpha \mid R_{\alpha\beta} \mid E\,\lambda_\beta \rangle_\beta \equiv {}_\alpha\langle \lambda_\alpha \mid R_{\alpha\beta}(E) \mid \lambda_\beta \rangle_\beta . \tag{3.5}$$

In all scattering problems of physical interest this operator is a bona fide integral operator.

The unitarity condition for the S matrix can now be expressed by the following relation

$$\begin{aligned}{}_\alpha\langle \lambda_\alpha \mid R_{\alpha\beta}(E) \mid \lambda_\beta \rangle_\beta + {}_\beta\langle \lambda_\beta \mid R_{\beta\alpha}(E) \mid \lambda_\alpha \rangle_\alpha^* + \sum_\gamma \int d\lambda_\gamma \, {}_\alpha\langle \lambda_\alpha \mid R_{\alpha\gamma}(E) \mid \lambda_\gamma \rangle_\gamma \\ \times \, {}_\beta\langle \lambda_\beta \mid R_{\beta\gamma}(E) \mid \lambda_\gamma \rangle_\gamma^* = 0\end{aligned} \tag{3.6}$$

This relation is the unitarity condition in the multichannel case. We shall now examine under what condition it is correct.

We first translate this relation into another equivalent form by using formula (2.20) of the preceding section

$${}_\alpha\langle \lambda_\alpha \mid R_{\alpha\beta}(E) \mid \lambda_\beta \rangle_\beta = \langle \lambda_\alpha \mid \Omega^{(\alpha)} R_{\alpha\beta} \Omega^{(\beta)*}(E) \mid \lambda_\beta \rangle . \tag{3.7}$$

For the $\Omega^{(\alpha)}$ which appear in this equation, we may choose any of the intertwining operators defined by (3.1). Let us choose for instance $\Omega_+^{(\alpha)}$. We then find

$$\begin{aligned}{}_\alpha\langle \lambda_\alpha \mid R_{\alpha\beta}(E) \mid \lambda_\beta \rangle_\beta &= \langle \lambda_\alpha \mid \Omega_+^{(\alpha)} (\Omega_-^{(\alpha)*} \Omega_+^{(\beta)} - \delta_{\alpha\beta}) \, \Omega_+^{(\beta)*} \mid \lambda_\beta \rangle \\ &= \langle \lambda_\alpha \mid \Omega_+^{(\alpha)} \Omega_-^{(\alpha)*} F_+^{(\beta)} - \delta_{\alpha\beta} F_+^{(\beta)} \mid \lambda_\beta \rangle .\end{aligned} \tag{3.8}$$

By using formula (2.20) we can drop the projection onto the range of $F_+^{(\beta)}$ on the right. Furthermore since $\Omega_-^{(\alpha)*} F_-^{(\beta)} = \delta_{\alpha\beta} \Omega_-^{(\alpha)*}$ we can replace the term $\Omega_+^{(\alpha)} \Omega_-^{(\alpha)*}$ by the sum over the channel index. In this way we obtain (using (2.21) and (2.22))

$$\langle \lambda_\alpha \mid S_+ - \delta_{\alpha\beta} \mid \lambda_\beta \rangle = {}_\alpha\langle \lambda_\alpha \mid R_{\alpha\beta} \mid \lambda_\beta \rangle_\beta$$

where

$$S_+ = \sum_\delta \Omega_+^{(\delta)} \Omega_-^{(\delta)*} \tag{3.9}$$

and where we define

$$\langle \lambda_\alpha \mid S_+ \mid \lambda_\beta \rangle \equiv \langle \lambda_\alpha \mid F_\alpha S_+ F_\beta \mid \lambda_\beta \rangle .$$

It is now easy to verify Equation (3.6), because it expresses the fact that the operator S_+ is unitary in the subspace $F\,\mathcal{H}$ with $F = \sum_\alpha F_\pm^{(\alpha)}$. It is thus equivalent with the equation

$$S_+^*\, S_+ = S_+\, S_+^* = F \equiv \sum_\alpha F^\alpha_{(\pm)}\,. \tag{3.10}$$

In order to verify this relation we substitute (3.9) into (3.10) and use the relations (3.2) and (3.3). Thus we obtain for instance

$$\begin{aligned} S_+^*\, S_+ &= \sum_\alpha \Omega_-^{(\alpha)}\, \Omega_+^{(\alpha)*} \sum_\beta \Omega_+^{(\beta)}\, \Omega_-^{(\beta)*} \\ &= \sum_{\alpha,\beta} \Omega_-^{(\alpha)}\, \delta_{\alpha\beta}\, E_\alpha\, \Omega_-^{(\beta)*} = \sum_\alpha \Omega_-^{(\alpha)}\, \Omega_-^{(\alpha)*} = \sum_\alpha F_-^{(\alpha)} = F \end{aligned}$$

and similarly

$$\begin{aligned} S_+\, S_+^* &= \sum_\alpha \Omega_+^{(\alpha)}\, \Omega_-^{(\alpha)*} \sum_\beta \Omega_-^{(\beta)}\, \Omega_+^{(\beta)*} \\ &= \sum_{\alpha,\beta} \Omega_+^{(\alpha)}\, \delta_{\alpha\beta}\, E_\alpha\, \Omega_+^{(\beta)*} = \sum_\alpha \Omega_+^{(\alpha)}\, \Omega_+^{(\alpha)*} = \sum_\alpha F_+^{(\alpha)} = F\,. \end{aligned}$$

Thus relation (3.10) is proved and with it the unitarity relation (3.6).

In order to obtain this last result we have used two properties of multichannel systems contained in the following two equations

$$\sum_\alpha F_+^{(\alpha)} = \sum_\alpha F_-^{(\alpha)} \tag{3.11}$$

and

$$F_\pm^{(\alpha)}\, F_\pm^{(\beta)} = \delta_{\alpha\beta}\, F_\pm^{(\alpha)}\,. \tag{3.12}$$

The property (3.11) is an essential hypothesis which scattering systems must satisfy if the S matrix is to be unitary [8]. It is independent of the asymptotic condition (3.1). The second relation (3.12) which states that the ranges for the different channels are pairwise orthogonal, on the other hand, is a consequence of the asymptotic condition and the fact that the spectra of the channel operators are continuous. This theorem was stated and proved in Ref. [8] (cf. Theorem on page 617).

We note here that the projections E_α do not satisfy any orthogonality relations. In fact one of these projections may be the identity operator as it is the case for instance in the example discussed in the first section. This lack of any orthogonality relation for the E_α is the cause of the overlapping channels.

Instead of working with the operator S_+ (3.9) we could also have used the operator S_- defined by

$$S_- = \sum_\delta \Omega_-^{(\delta)}\, \Omega_+^{(\delta)*} \tag{3.13}$$

which would have appeared instead of S_+ if we had chosen the spectral representation (3.7) with the operators $\Omega_-^{(\alpha)}$ instead of $\Omega_+^{(\alpha)}$ as we have done from Equation (3.8) on. Although the ranges of $F_\pm^{(\alpha)}$ are different for the two signs, the result would have been identical, since we would have obtained again a spectral representation of the operator relation

$$S_-^* \, S_- = S_- \, S_-^* = F \tag{3.14}$$

which is proved similarly to (3.10).

The unitarity of the S matrix is thereby proved even for rearrangement collisions with overlapping channels.

IV. Conclusion

We have succeeded in proving the unitarity relation of the S matrix for rearrangement collisions on the basis of the following three hypotheses:

(1) There exists a *self-adjoint evolution* operator H for the entire scattering system which generates the unitary group $V_t = e^{-iHt}$.

(2) Each channel is characterized by an *asymptotic condition*, which defines a self-adjoint channel operator H_α, representing the *kinetic energy* of the channel fragments, and which implies the existence of the limits

$$\Omega_\pm^{(\alpha)} = \lim_{t \to \mp\infty} V_t^* \, U_t^{(\alpha)}$$

with

$$U_t^{(\alpha)} = e^{-iH_\alpha t} .$$

(3) The projections $F_\pm^{(\alpha)}$ onto the ranges of the operators $\Omega_\pm^{(\alpha)}$ satisfy

$$\sum_\alpha F_+^{(\alpha)} = \sum_\alpha F_-^{(\alpha)} .$$

The physical interpretations of these conditions is the following: (1) says that the evolution of the states is the unfolding of a continuous symmetry transformation of the system. It is equivalent with the existence of a Schrödinger equation; (2) expresses the physical content of a scattering process and (3) says that every state in the continuum part of H is a scattering state.

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