Theory of the scattering operator

Jauch, Joseph-Maria

Theory of the scattering operator*)

by **J. M. Jauch**

Department of Physics, State University of Iowa, Iowa City, Iowa

(17. XI. 1957)

Abstract. In this paper we give a complete theory of the scattering operator on a rigorous mathematical foundation for a certain class of quantum mechanical systems called, 'simple scattering systems'. These systems are characterized by three properties formulated in Section 3. The relation of these properties to the physical content of scattering is explained. We then proceed to define the wave operator and the scattering operator and prove their existence with mathematically rigorous methods. No assumptions are needed regarding the occurrence of bound states and the location of their energy with respect to the continuum region of the total energy operator. In Section 4 we demonstrate the existence of a certain integral representation of the scattering operator which has often been used as a starting point of the iteration approximation. Certain general properties of scattering systems are obtained in Section 5. This leads to necessary conditions for systems to be scattering systems as well as to a new definition of the scattering operator. The paper concludes with a derivation of the scattering cross-section from the scattering operator. The improvement of this derivation over the older ones consists in the special care employed for stating the assumptions which must go into such a derivation and the avoidence of improper functions or other artificial devices.

1. Introduction

It is generally recognized that the scattering operator is one of the most fundamental concepts in elementary wave mechanics as well as in relativistic field theories. Yet a mathematically meaningful definition of this operator does not seem to be known. It is the purpose of this paper to supply such a definition and to prove the existence of this operator under certain assumptions which characterize the scattering systems.

All the 'definitions' usually employed are of a purely formal character based on a mathematical formalism which is simply derived from the analogy between the Hilbert space and the finite-dimensional vector spaces. These analogies exist but only to a limited extent and for the questions centering around the concept of the scattering operator the properties, for which this analogy fails, are the most important ones.

There has been a widely felt need for a satisfactory treatment of the mathematical theory of scattering. However, all recent attempts in this

*) Supported by the National Science Foundation.

direction have fallen short of this objective and have remained inconclusive and heuristic in character[1–10] *).

In order to make any progress in the mathematical scattering theory it seemed to us essential to approach these problems with a new standard of rigor and with mathematical methods of a more recent vintage than the ones now generally employed by theoretical physicists. We hope that this approach will eventually throw some light on many of the questions in relativistic field theories which hitherto have been obscured by the lack of rigor generally prevailing in theoretical physics.

The main problem in such an endeavor has been to reformulate the physical scattering process in terms of a meaningful mathematical language. The commonly employed method of representing scattering states by non-normalizable wave functions leads to difficulties because it does not seem possible to introduce a suitable topology in a function space which contains these wave functions[11]). Under such circumstances the studying of limiting properties becomes exceedingly complicated.

We have, therefore, abandoned this approach and have developed a scattering theory in which the states of the physical system are represented by the elements of a Hilbertspace consisting of L^2-functions in a suitable domain. Besides the mathematical reasons there are good physical reasons why we believe this to be desirable. The matrix elements of such functions have a direct and simple physical interpretation as the probability amplitudes for the result of certain measurements. This interpretation is lost in the function spaces of larger extent than the L^2-space. It can only be reintroduced by certain artificial devices, such as very large boxes or the consideration of an infinite assembly of identical systems. The artificiality of these devices merely exemplifies the inadequacy of the mathematical description.

In order to keep the mathematical language meaningful throughout it is essential to refrain from using improper functions, such as the Dirac δ-function, and it is necessary to pay full attention to the domain of linear operators and in the study of limiting relations the underlying topology must be specified.

As regards the δ-function, we are aware that in many instances its use is a convenient and in most cases harmless symbolic notation for a sometimes cumbersome limiting relation. However, this is not always the case and the indiscriminate use of this device has obscured the mathematical difficulties which still beset the general field theories. Besides, there is

*) *Note added in proof:* The interesting paper by J. M. Cook, Journ. of Math. and Phys. **36**, 81 (1957) has just come to our attention. It is a notable exception to the above statement. According to this paper any system with a square integrable interaction potential is a "simple scattering system" as defined in this paper.

really no good reason to retain this mathematical fiction invented at a time when the mathematics of Hilbert space and functional analysis was little known to physicists. This well developed and easily accessible branch of mathematics contains most of the tools needed for handling the mathematical problems involved in the theory of scattering.

In the present paper we restrict ourselves to a rather simple class of scattering systems for which the existence problem can be rigorously formulated and solved. This class contains the wave-mechanical scattering systems involving only one single channel but it excludes so far all reaction processes such as they occur in nuclear collisions and in particle creation and annihilation processes. The formulation is of sufficient latitude to allow the necessary generalizations to the cases of scattering with a finite number of channels. The cases involving infinitely many channels such as they occur in field theory are much more difficult to treat and lead to mathematical problems which have not even been properly formulated at the present time.

Even within the limitations which we have imposed we need certain mathematical results in the theory of functional analysis. Since these are not generally known by physicists to which this paper addresses itself primarily, we have given in section 2 a very brief review of some of the definitions and theorems (without proofs) which are used in the rest of the paper.

2. Mathematical Preliminaries

In this section we shall give some of the basic definitions as well as some of the more important theorems needed in the rest of the paper[13]).

The statevectors of a physical system are in one-to-one correspondence with the normalized elements of a Hilbert space $\mathfrak{H}$. This space is usually realized in terms of the quadratically integrable functions on a Euclidean space of finite dimensions. For the intrinsic properties of the Hilbert space its particular realization by such functions is not essential and we can therefore express them in the abstract form in which no reference is made to such a realization.

A Hilbert space is a set of elements, denoted by $f, g \ldots$, which satisfy the following properties:

(1) They form a linear vectorspace over the complex numbers.
(2) There exists a positive definite scalar product.
(3) The space is complete.
(4) The space is separable.

The first two properties are so well-known that very little comment is needed. We merely mention that the scalar product between two elements $f, g \in \mathfrak{H}$ will be denoted by (f, g). The scalar product serves to intro-

duce a *metric* in $\mathfrak{H}$. The *distance* between two elements $f, g \varepsilon \mathfrak{H}$ is the positive square root

$$\| f - g \| = \sqrt{((f - g), (f - g))} .$$

The following inequalities will be frequently used

$$| (f, g) | \leqslant \| f \| \, \| g \| ,$$
$$\| f + g \| \leqslant \| f \| + \| g \| .$$

Properties (3) and (4) are automatically satisfied for finite-dimensional vectorspaces and it is for this reason that physicists usually pay no attention to them*).

Roughly speaking condition (3) ensures that the space is large enough while (4) ensures that it is not too large. Condition (3) can be explained most easily in terms of fundamental sequences:

A sequence $\{f_n\}$ of elements $f_n \varepsilon \mathfrak{H}$ is a *fundamental sequence* if for each $\varepsilon > 0$ there exists an N such that

$$\| f_n - f_m \| < \varepsilon \quad \text{for all} \quad n, m > N .$$

Condition (3) states that every fundamental sequence has a limit. Thus if $\{f_n\}$ is such a sequence then there exists an element $f \varepsilon \mathfrak{H}$ with the property: For all $\varepsilon > 0$ one can select a positive integer N, such that

$$\| f - f_n \| < \varepsilon \quad \text{for all} \quad n > N .$$

The limit concept used here refers to the so-called *strong topology* in $\mathfrak{H}$ There is another type of limit which defines a *weak topology:* f_n converges weakly to f, in symbols

$$f \rightharpoonup f_n \quad \text{for} \quad n \to \infty$$

if

$$(g, f_n) \to (g, f) \quad \text{for all} \quad g \varepsilon \mathfrak{H} .$$

Strong convergence always implies weak convergence but *not* vice versa. We shall work almost exclusively with the strong topology and strong limits will always be implied unless a statement to the contrary is made.

If M is a subset of elements in $\mathfrak{H}$ we can add to M all its limit points and obtain its closure $\overline{M}$. Obviously $M \subset \overline{M}$ and $\overline{\overline{M}} = \overline{M}$. Property (4) says that there exists a countable subset M of $\mathfrak{H}$ such that

$$\overline{M} = \mathfrak{H} .$$

Property (4) is always satisfied for the elementary systems in Quantum

*) It may be noted that we have not introduced a dimension axiom as it is often done for the Hilbert space. Hence all finite dimensional spaces are included in this definition. For quantum mechanical systems this is often convenient.

Mechanics but is *not satisfied* for the systems described by a quantized field theory. When (4) is not satisfied we refer to a non-separable Hilbert space. The fact that (4) is violated for field theories is one of the main obstacles for a theory of the scattering operator in these cases.

The following concepts will be used frequently throughout the rest of this paper but they will not be explained.

Linear manifolds and closed linear manifolds (the latter are also called subspaces), orthogonal complements, projection operators, orthogonal systems and complete orthogonal systems, bounded and unbounded linear operators domains of definition, unitary and self-adjoint operators.

These concepts are explained in detail in any of the mentioned references.

We shall state two theorems on functionals which have been found useful in connection with our problem. We precede them by two definitions:

A function $\Phi(f)$ with domain $\mathfrak{H}$ and values in the complex numbers C is called a *linear functional* if it satisfies the following two properties:

$$\Phi(\lambda f + \mu g) = \lambda \Phi(f) + \mu \Phi(g); \quad \lambda, \mu \varepsilon C; \quad f, g \varepsilon H . \tag{a}$$

$$| \varphi(f) | \leqslant A \| f \| \quad A \text{ fixed } > 0 . \tag{b}$$

A function $\Phi(f, g)$ with domain $\mathfrak{H} \times \mathfrak{H}$ (the topological product of $\mathfrak{H}$ with itself) and values in the complex numbers C is called a *bilinear functional* if it satisfies the following three properties:

$$\Phi(\lambda_1 f_1 + \lambda_2 f_2, g) = \lambda_1^* \Phi(f_1, g) + \lambda_2^* \Phi(f_2, g) \tag{a}$$

$$\Phi(f, \mu_1 g_1 + \mu_2 g_2) = \mu_1 \Phi(f, g_1) + \mu_2 \Phi(f, g_2) \tag{b}$$

$$|\Phi(f, g) | \leqslant B \| f \| \, \| g \| , \quad B \text{ fixed} > 0 . \tag{c}$$

The two theorems are: Every linear functional $\Phi(f)$ is of the form

$$\Phi(f) = (g, f)$$

with some fixed $g \varepsilon \mathfrak{H}$ (RIESZ-FRÉCHET). For every bilinear functional $\Phi(f, g)$ there exists a bounded linear operator A such that

$$\Phi(f, g) = (f, A g) .$$

The bound of A is given by

$$\| A \| = \underset{f, g \varepsilon \mathfrak{H}}{l. \text{u. } b.} \frac{\Phi(f, g)}{\| f \| \, \| g \|} \equiv \| \Phi \| .$$

The second theorem is a simple consequence of the first.

We further need the spectral theorems for the selfadjoint and unitary operators. The following definition is used in this connection:

A family of projection operators $E(\lambda)$ (λ real) is said to be *non-decrasing* with λ if for every $f \varepsilon \mathfrak{H}$

$$(f, E(\lambda_1) f) \leqslant (f, E(\lambda_2) f) \text{ for } \lambda_1 \leqslant \lambda_2 ;$$

we write

$$E(\lambda_1) \leqslant E(\lambda_2) .$$

The spectral theorem for self adjoint operators may now be stated as follows: To every self-adjoint operator A there exists a non-decreasing family of projection operators such that

$$E(-\infty) = 0 , \quad E(+\infty) = I$$

and

$$A = \int_{-\infty}^{+\infty} \lambda \, d E(\lambda) .$$

In this expression the integral is to be interpreted as the Stieltjes integral valid for any pair of elements $f, g \varepsilon \mathfrak{H}$:

$$(f, A g) = \int_{-\infty}^{+\infty} \lambda \, d(f, E(\lambda) g) .$$

The spectral representation is most useful for the definition of the functions of a self-adjoint operator. If $F(\lambda)$ is a function of the real variable λ the function $F(A)$ is defined as

$$F(A) = \int_{-\infty}^{+\infty} F(\lambda) \, dE(\lambda) .$$

The domain of definition $D_{F(A)}$ is the linear manifold of all $f \varepsilon \mathfrak{H}$ for which

$$\int_{-\infty}^{+\infty} |F(\lambda)|^2 \, d(f, E(\lambda) f) < \infty .$$

We shall be dealing primarily with unitary operator families U_t depending on a parameter t and expressible in terms of a self-adjoint operator A as an exponential function

$$U_t = e^{iAt} \quad (t \text{ real}) .$$

It follows from the above definition that

$$U_t = \int_{-\infty}^{+\infty} e^{i\lambda t} \, dE(\lambda)$$

and that the domain of definition of U_t is the whole of $\mathfrak{H}$. The operator family U_t satisfies

$$U_t U_s = U_{t+s} = U_s U_t$$

and it is a *representation* of the additive group of real numbers.

Two self-adjoint operators A and B are said to be unitarily equivalent if there exists a unitary operator X such that the domains of B and XAX^{-1} are equal and that throughout this domain $Bf = XAX^{-1}$. If $E(\lambda)$ and $F(\lambda)$ are the spectral families of A and B then

$$F(\lambda) = X\, E(\lambda)\, X^{-1}$$

for all λ. It follows from this that the corresponding operators $U_t = e^{iAt}$ and $V_t = e^{iBt}$ are also unitarily equivalent, that is

$$V_t = X\, U_t\, X^{-1}$$

for all t. In this case we also write $V_t \simeq U_t$. This is an equivalence relation.

In the fifth section we shall have occasion to introduce subspaces invariant under a unitary group representation such as U_t. A set $M \subset \mathfrak{H}$ is said to be a subspace invariant under U_t if it is a closed linear manifold and if for any $f \in M$, $U_t f \in M$ for all t.

If $N = M^{\perp}$ is the orthogonal complement of M and M is an invariant subspace then N is too.

If E_M and E_N are the projection operators corresponding to these two subspaces, such that

$$E_M E_N = E_N E_M = 0$$

$$E_M + E_N = I\,,$$

then

$$U_t E_M = E_M U_t \equiv {}^M U_t\,.$$

and

$$U_t E_N = E_N U_t \equiv {}^N U_t\,.$$

The representations ${}^M U_t$ and ${}^N U_t$ are said to be the *reduction* of U_t to M and N respectively. We always have

$${}^M U_t + {}^N U_t = U_t$$

and we say U_t is *decomposed*. The representations ${}^M U_t$ and ${}^N U_t$ are called *subrepresentations* of U_t.

If U_t is equivalent to some subrepresentation ${}^M V_t$ of V_t then we say U_t is *contained* in V_t. We use the notation $U_t \lesssim V_t$ for this situation.

3. Definition of a Scattering System

The dynamical properties of a quantum mechanical system are contained in the structure of a self-adjoint linear operator H operating in a separable Hilbert space $\mathfrak{H}$. The operator represents the total energy of the system. In the more interesting systems H is an unbounded operator. However, in all systems the energy has a *lower* bound. An operator with this property is called *semi-bounded*. The mathematical expression for this is

$$(f, H f) \geqslant 0 \qquad \text{for} \quad f \varepsilon D_H . \tag{3.1}$$

Here D_H is the domain of definition of H which is everywhere dense in $\mathfrak{H}$ and we have arbitrarily put the lower bound of H equal to zero which is no restriction since an additive constant in H can always be adjusted without changing the physical content of the system.

We wish to introduce now additional restrictions on H which select from the class of all quantum mechanical systems a certain subclass which we shall call the *scattering systems*.

In order to motivate these restrictions we shall for a moment digress to the intuitive description of a scattering process. Such a process must be visualized essentially in three stages. In the first stage we have a number of incident particles (in practice either one or two) approaching each other (or in the case of one particle, approaching the scatterer). In the second stage which lasts only a very short time compared with the duration of the whole process a collision occurs. After the collision a number of particles emerge with their direction of motion different from the original direction. This is the third stage.

This intuitive picture is at the basis of the theory of scattering. The problem is to find the adequate mathematical language for the expression of this physical situation. In the description which we have given we have not made the assumption that the numbers or even the kind of particles are the same before and after the collision process, nor have we implied anything concerning internal degrees of freedom such as a spin or isotopic spin for the particles partaking in the scattering process. The mathematical description should be sufficiently broad so as to include these cases.

The essential feature of the scattering process is that in the remote past and in the distant future the motion of the particle is 'free'. This means that in the limit $t \to \pm \infty$ no interaction between the particles is operating. The time development of such 'free' particles is governed by a 'free' Hamiltonian which represents the total kinetic energy of the participating particles. These free Hamiltonians H_α depend on the number and kind of incident or emerging particles. They always have either one

of the following forms, depending on whether we treat the particles relativistically or not.

$$H_\alpha = \sum_\nu \frac{1}{2m_\nu} \boldsymbol{p}_\nu^2 , \tag{3.2}$$

$$H_\alpha = \sum_\nu \sqrt{m_\nu^2 + \boldsymbol{p}_\nu^2} . \tag{3.3}$$

Here $\boldsymbol{p}_\nu$ represents the momentum operator of the particle, m_ν its mass. The operators $\boldsymbol{p}_\nu$ are self-adjoint and the positive square root in (3.3) is defined in the manner as indicated in the preceding section. The index α distinguishes the various kinds and numbers of particles which can participate in the scattering process and it is called the *channel index*. Whichever form of H_α is adopted, these operators are always semi-bounded self-adjoint linear operators such that

$$(f, H_\alpha f) \geqslant 0 \qquad (f \varepsilon D_{H_\alpha}) . \tag{3.4}$$

In order to simplify the mathematical formulation we shall restrict ourselves in this paper to the case of only one channel. We speak then of a single channel scattering and the system is called a 'simple' scattering system. The corresponding free Hamiltonian will be denoted by H_0. The number of particles participating in the collision is either one or two and it is the same before and after the collision. Instead of the operators H_0 and H it is more convenient to introduce the unitary operators U_t and V_t defined by

$$\begin{aligned} U_t &= e^{-iH_0 t} \\ V_t &= e^{-iHt} . \end{aligned} \tag{3.5}$$

The unitary property is expressed by

$$\begin{aligned} U_t^* &= U_{-t} \\ V_t^* &= V_{-t} . \end{aligned} \tag{3.6}$$

The advantage of the operators U_t and V_t is that they are defined everywhere in $\mathfrak{H}$ while H_0 and H are only defined in everywhere dense linear manifolds. It is then not necessary to indicate the domain of definition of these operators and they can be freely multiplied without restrictions since the range of one is always contained in the domain of the other.

In the usual formulation of scattering theory the initial and final states are always represented in the form of plane waves and these are called 'eigen states' of the operator H_0.

It is here that our formulation of the scattering theory departs from the usual one. The spectrum of the operator H_0 is always continuous, hence *there exist no* 'eigen states' in the underlying Hilbert space.

The correct formulation of initial and final states is in terms of *wave packets*, that is, elements $f \varepsilon \mathfrak{H}$. This formulation, incidentally, corresponds much closer to the actual physical situation than the plane-wave representation which is physically an abstraction and mathematically most inconvenient because plane-waves are not contained in $\mathfrak{H}$.

The first condition which is necessary for a system to be a scattering system is that the limits

$$\lim_{t \to \mp \infty} V_t^* U_t f = f_\pm \tag{I}$$

exist*) for all $f \varepsilon \mathfrak{H}$.

The set of elements which are limits in the sense of (I) are denoted by $R_\pm$. The second condition which we require is that these two sets are identical:

$$R_+ = R_- = R\,. \tag{II}$$

We shall now show that these conditions contain the essential ingredients of the usual formulation of the scattering theory. The elements of the form

$$f_+ = \lim_{t \to -\infty} V_t^* U_t f$$

are those states which in the usual presentation of scattering theory are represented by 'plane waves' plus 'outgoing scattered waves'. Similarly the f_- correspond to 'plane waves' plus 'ingoing scattered waves'. The significance of the limits (I) can be illuminated by the following remarks: If the limit I exists, then, for instance, the limit

$$\lim_{t \to -\infty} U_t^* V_t f_+ = f \tag{3.7}$$

exists also. This may be seen as follows: (I) means that for $\varepsilon > 0$, arbitrary, there exists a T such that

$$\| V_t^* U_t f - f_+ \| < \varepsilon$$

for all $t > T$, since V_t and U_t are unitary we also have

$$\| V_t^* U_t f - f_+ \| = \| f - U_t^* V_t f_+ \| < \varepsilon$$

for the same t.

The vector $g(t) = U_t^* V_t g$ has a familiar interpretation. It represents a state of the system in the *interaction picture* when g represents that same state in the *Heisenberg picture*. Hence the existence of this limit

*) The existence of the limit $t \to + \infty$ can be proved if the limit $t \to - \infty$ exists and vice versa if an additional assumption is made expressing invariance of the system under the time reversal transformation. This point will be elaborated elsewhere and will not be persued further here.

means that the state in the interaction picture approaches a constant as $t \to -\infty$. Now in the interaction picture the states change only because of the interaction operator $H - H_0$. The fact that these states approach a constant means that the interaction becomes ineffective for the remote past. Because of condition (II) a similar statement holds for the limit $t \to +\infty$. This is precisely the physical property we mean to imply with a scattering system.

To the two conditions we shall add a third condition which we shall take as characterizing the *simple scattering systems*. In order to formulate this condition we define the subspace M consisting of the closed linear manifold spanned by the proper elements of H, that is, all elements of the form

$$H f = \omega f \qquad (\omega \text{ real}) .$$

The orthogonal complement $M^{\perp}$ of M is denoted by N and elements in N are said to belong to the continuum of H. The third condition then requires that

$$N \mathbf{C} R . \tag{III}$$

We shall prove in the next section that always $R \mathbf{C} N$. Hence (III) can also be replaced by $N = R$. The meaning of this condition is that there are no states in the continuum of H which are not scattering states associated with H_0. If there were such states the description of the scattering states in terms of H and H_0 alone would be incomplete. This is precisely the situation in the multichannel scattering processes; hence we shall adopt condition (III) as characterizing the simple scattering systems.

We shall now derive a few simple conclusions from these properties of scattering systems. The mapping $f \to f_{\pm}$ of $\mathfrak{H}$ onto R is a linear mapping and an isometry. The linear property of the mapping is obvious. We verify the isometry: $\| f \| = \| f_{\pm} \|$.

Since $\| V_t^* U_t f \| = \| f \|$ the left-hand side is independent of t. Hence in the limit

$$\| f \| = \| f_{\pm} \|$$

We can therefore introduce a pair of bounded linear aperators $\Omega_{\pm}$ defined in all of $\mathfrak{H}$ and with range R such that

$$\Omega_{\pm} f = f_{\pm} \quad \text{or} \quad \Omega_{\pm} = \lim_{t \to \mp\infty} V_t^* U_t \tag{3.8}$$

the bound of $\Omega_{\pm}$ is $\| \Omega_{\pm} \| = 1$. These operators will be called the 'wave-operators'. Since Ω is isometric R is a subspace.

*

Let Ω be either one of the wave-operators. Since Ω is bounded and defined everywhere we can define everywhere in $\mathfrak{H}$ the adjoint operator Ω^* as a bounded linear operator with the defining property

$$(\Omega^* f, g) = (f, \Omega g) . \tag{3.9}$$

for all $g \varepsilon \mathfrak{H}$. Let Q be the set of elements $f \varepsilon \mathfrak{H}$ such that

$$\Omega^* f = 0 . \tag{3.10}$$

From the defining property (3.9) it follows immediately that $f \varepsilon Q$ implies $f \varepsilon R^\perp$ (the orthogonal complement of R). Similarly if $f \varepsilon R^\perp$ then $(\Omega^* f, g) = 0$ for all g or $\Omega^* f = 0$ that is $f \varepsilon Q$. Thus $Q = R^\perp$. On the other hand if $f \varepsilon R$ then there exists a $g \varepsilon \mathfrak{H}$ such that $\Omega g = f$. Hence because of (3.8) $\Omega^* f = \Omega^* \Omega g = g$. Thus the operator $\Omega\Omega^*$ is defined everywhere and it is the projection operator E_R with respect to R

$$\Omega_\pm \Omega_\pm^* = E_R = I - E_Q , \tag{3.11}$$

and

$$\Omega_\pm^* \Omega_\pm = I .$$

The projection E_Q may be called the *unitary deficiency* of the wave operator.

It is important to note that the right-hand side is independent of the sign attached to Ω. This is an important consequence of condition (II). A further property of the projection E_Q may be noted. Because of the definition (3.10) of Q we have

$$\Omega_+^* E_Q = \Omega_-^* E_Q = E_Q \Omega_- = E_Q \Omega_+ = 0 .$$

From this follows immediately that the operator

$$S = \Omega_-^* \Omega_+ \tag{3.12}$$

is unitary. Indeed

$$S^* S = \Omega_+^* \Omega_- \Omega_-^* \Omega_+ = \Omega_+^* (I - E_Q) \Omega_+ = \Omega_+^* \Omega_+ = I$$

and

$$SS^* = \Omega_-^* \Omega_+ \Omega_+^* \Omega_- = \Omega_-^* (I - E_Q) \Omega_-^* \Omega_- = I .$$

The unitary operator (3.12) is the scattering operator.

4. Integral Representations of the Wave Operator

In a previous publication we have given explicit integral representations of the operators $\Omega_\pm$ which can be made the starting point of certain approximation methods for determining these operators[1]. These representations were purely formal in character and a proof of their existence has never been given. In this section we shall give such an existence proof for the case of simple scattering systems.

We begin by stating and proving a few lemmata.

Lemma 1. The elements $U_t f$ and $V_t f$ are strongly continuous functions of the real variable t for all t and all $f \varepsilon \mathfrak{H}$.

Proof: Strong continuity of $U_t f$ at $t = t_0$ means that for $\varepsilon > 0$, there exists a $\delta > 0$ such that

$$\| U_t f - U_{t_0} f \| < \varepsilon \quad \text{for } | t - t_0 | < \delta . \tag{4.1}$$

Because of the group property and the unitary property of U_t this is equivalent to continuity at $t = 0$:

$$\| (I - U_t) f \| < \varepsilon \quad \text{for } | t | < \delta . \tag{4.2}$$

This expression can be put into a slightly more convenient form by writing

$$\| (I - U_t) f \| = \sqrt{((I - U_t) f, (I - U_t) f)} = \sqrt{(f, (2 - U_t - U_{-t}) f)} . \tag{4.3}$$

Since $U_t = e^{-iH_0 t}$, and H_0 is self adjoint, there exists a sequence of non-decreasing projection operators $E(\lambda)$ $(-\infty < \lambda < +\infty)$ such that

$$E(-\infty) = 0 , \qquad E(+\infty) = I \tag{4.4}$$

and

$$(f, U_t f) = \int_{-\infty}^{+\infty} e^{-i\lambda t} \, d(f, E(\lambda) f) . \tag{4.5}$$

When this is substituted in (4.3) and (4.4) is used we obtain

$$\| (1 - U_t) f \| = 2 \left[\int_{-\infty}^{+\infty} \sin^2 \frac{\lambda t}{2} \, d(f, E(\lambda) f) \right]^{1/2} . \tag{4.6}$$

Since the function $[f, E(\lambda) f]$ is monotonically increasing with λ we can majorize the integral by replacing $\sin^2 \lambda t/2$ by the larger value $\lambda^2 t^2/4$

$$\| (1 - U_t) f \| \leqslant t \left[\int_{-\infty}^{+\infty} \lambda^2 \, d(f, E(\lambda) f) \right]^{1/2} . \tag{4.7}$$

Thus if f is in the domain of H_0

$$\| (1 - U_t) f \| \leqslant t \cdot C \tag{4.8}$$

where

$$C = \| H_0 f \|$$

is some fixed positive number. If $g \varepsilon \mathfrak{H}$ is an arbitrary element then, using

the fact that the domain of H_0 is everywhere dense in $\mathfrak{H}$, we can find an $f \varepsilon D_{H_0}$ such that

$$\| g - f \| < \frac{\varepsilon}{4}$$

with this f fixed we select $t < \varepsilon/2\,C = \delta$ and obtain

$$\| (1 - U_t)\, g \| \leqslant \| (1 - U_t)\, (g - f) \| + \| (1 - U_t)\, f \|$$

$$\leqslant 2 \cdot \frac{\varepsilon}{4} + \frac{\varepsilon}{2} = \varepsilon, \text{ q. e. d.}$$

The proof is equally valid for V_t provided we replace H_0 by H.

Lemma 2. Let $W_t = V_t^* U_t$, then the function $W_t f$ is strongly continuous for all t and all $f \varepsilon \mathfrak{H}$.

Proof: Let t_0 be some fixed value of t and write

$$W_t - W_{t_0} = V_t^* (U_t - U_{t_0}) + (V_t^* - V_{t_0}^*)\, U_{t_0}$$

$$\| (W_t - W_{t_0})\, f \| \leqslant \| (U_t - U_{t_0})\, f \| + \| (V_t^* - V_{t_0}^*)\, g \|$$

where

$$g = U_{t_0} f .$$

Strong continuity of $W_t f$ at $t = t_0$ now follows from lemma 1, q. e. d.

Lemma 3. The function $\varphi(t) \equiv (f, W_t\, g)$ is continuous for all t and all $f, g \varepsilon \mathfrak{H}$ and $| \varphi(t) | \leqslant \| f \| \| g \|$.

Proof: Strong continuity implies weak continuity which is the statement of the lemma 3. The boundedness follows from the fact that W_t is unitary and therefore

$$| \varphi (t) | = | (f, W_t\, g) | \leqslant \| f \| \ \| W_t\, g \| = \| f \| \ \| g \| , \tag{4.9}$$

Lemma 4. The integral

$$\Phi_\varepsilon (f, g) = \varepsilon \int_0^\infty e^{-\varepsilon t} \varphi (t)\, dt \tag{4.10}$$

where $\varphi(t) = (f, W_t\, g)$, is absolutely convergent for all $f, g \varepsilon \mathfrak{H}$ and $\varepsilon > 0$ and it is bounded:

$$| \Phi_\varepsilon (f, g) | \leqslant \| f \| \ \| g \| . \tag{4.11}$$

Proof: The integrand is continuous and hence integrable on any finite interval. The absolute convergence follows from the boundedness of $\varphi(t)$ (lemma 3)

$$| \Phi_\varepsilon (f, g) | \leqslant \varepsilon \int_0^\infty e^{-\varepsilon t} | \varphi (t) | dt \leqslant \varepsilon \int_0^\infty e^{-\varepsilon t} \| f \| \ \| g \| = \| f \| \| g \|, \text{ q. e}$$

It follows from the last lemma and the obvious bilinear property of $\Phi_\varepsilon(f, g)$ that it is a bilinear functional with upper bound 1. (For the definition, see Section 2). According to the theorem quoted in Section 2 there exists a linear operator Ω_ε with the property

$$\Phi_\varepsilon(f, g) = (f, \Omega_\varepsilon g) \qquad (4.12)$$
$$\| \Omega_\varepsilon \| \leqslant 1 .$$

The operator thereby defined may be written as

$$\Omega_{-\varepsilon} = \varepsilon \int_0^\infty e^{-\varepsilon t} V_t^* U_t \, dt \qquad (\varepsilon > 0) . \qquad (4.13)$$

There is a corresponding operator defined by

$$\Omega_{+\varepsilon} = \varepsilon \int_{-\infty}^0 e^{\varepsilon t} V_t^* U_t \, dt \qquad (\varepsilon > 0) . \qquad (4.14)$$

When the distinction between the two operators is irrelevant we shall omit the $\pm$ and denote one of the two cases simply by Ω_ε.

Our next task is to study the limit $\varepsilon \to +0$ for the operators Ω_ε. The limit of a set of operators can be understood in three senses:

(1) *The limit in the norm:* Ω_ε converges in the norm to Ω ($\Omega_\varepsilon \Longrightarrow \Omega$) if

$$\| \Omega_\varepsilon - \Omega \| \to 0 .$$

(2) *The strong limit:* Ω_ε converges strongly to Ω ($\Omega_\varepsilon \to \Omega$) on a subset $M \varepsilon \mathfrak{H}$ if for all $f \varepsilon M$

$$\| (\Omega_\varepsilon - \Omega) f \| \to 0 .$$

(3) *The weak limit:* Ω_ε converges weekly to Ω ($\Omega_\varepsilon \rightharpoonup \Omega$) on a subset $M \varepsilon \mathfrak{H}$ if for all $f, g \varepsilon M$

$$| (f, \Omega_\varepsilon g) - (f, \Omega g) | \to 0 .$$

One can show that (1) implies (2) and (2) implies (3), but the implications are not reversible. We shall understand our limits in the sense (2). We shall first prove the

Lemma 5. The set $L = \{f | \lim_{\varepsilon \to +0} \Omega f \text{ exists}\}$ is a closed linear manifold and $\lim_{\varepsilon \to +0} \Omega_\varepsilon$ is a bounded linear operator on M with bound $\leqslant 1$.

Proof: That L is a linear manifold follows from the fact that Ω_ε is a linear operator and that the limit of sums is the sum of the limits. That it is closed may be seen as follows:

Let $\{f_n\}$ be a sequence such that $f_n \to f$ and $f_n \varepsilon L$.

$$\| (\Omega_{\varepsilon_1} - \Omega_{\varepsilon_2}) f \| \leqslant \| (\Omega_{\varepsilon_1} - \Omega_{\varepsilon_2}) f_n \| + \| \Omega_{\varepsilon_1} (f - f_n) \| + \| \Omega_{\varepsilon_2} (f_n - f) \| . \qquad (4.15)$$

We chose $\delta > 0$ arbitrary and select an n such that

$$\| f - f_n \| < \frac{\delta}{3} .$$

and a pair ε_1, ε_2 such that for the aforementioned fixed n

$$\| (\Omega_{\varepsilon_1} - \Omega_{\varepsilon_2}) f_n \| < \frac{\delta}{3} .$$

Using the boundedness of Ω_ε we find from (4.15)

$$\| (\Omega_{\varepsilon_1} - \Omega_{\varepsilon_2}) f \| < \delta .$$

Since δ was arbitrary, $\lim_{\varepsilon \to +0} \Omega_\varepsilon f = \Omega f$ exists which shows that L is closed, q.e.d. The bound of $\lim \Omega_\varepsilon$ is

$$\text{l. u. b.}_{f \varepsilon M} \frac{\| \lim_{\varepsilon \to +0} \Omega_\varepsilon f \|}{\| f \|} \leqslant \lim_{\varepsilon \to +0} \int_0^\infty e^{-\varepsilon t} \| U_t^* V_t^* \| \, dt = \mathbf{1} .$$

Our next problem is to determine the extent of the space L. Lemma 5 shows that the set of elements f for which this limit exists is a subspace $L \subset \mathfrak{H}$. The operator $\Omega \equiv \lim_{\varepsilon \to +0} \Omega_\varepsilon$ is therefore defined throughout L and is there a bounded linear operator with bound $\| \Omega \| \leqslant 1$. We could always extend the definition of Ω to a bounded operator in all of $\mathfrak{H}$ which in L agrees with Ω and which has the same bound as Ω by the following procedure. Let $L^\perp$ be the orthogonal complement of L and write for any $f \varepsilon \mathfrak{H}$ the unique decomposition

$$f = f_1 + f_2 \quad f_1 \varepsilon L , \quad f_2 \varepsilon L^\perp$$

l. c. then the assignment $f \to \Omega f_1$, is a proper extension of Ω with the same bound.

We shall see, however, that for scattering systems there is no need to do so, since for such systems the $\lim \Omega$ exists throughout all of $\mathfrak{H}$. This is an immediate consequence of the following.

Lemma 6:

$$\text{If } \lim_{t \to +0} V_t^* U_t f = f_- \text{ exists then}$$

$$\lim_{\varepsilon \to +0} \varepsilon \int_0^\infty e^{-\varepsilon t} V_t^* U_t f \, dt$$

exists also and it is equal to f_- .

Proof: Let $f_- = \lim_{t \to +\infty} V_t^* U_t f$. Then

$$\| \varepsilon \int_0^\infty e^{-\varepsilon t} V_t^* U_t f \, dt - f_- \| \leqslant \int_0^\infty e^{-\tau} \| V_{\tau/\varepsilon}^* U_{\tau/\varepsilon} f - f_- \| \, d\tau .$$

The integral on the right may be separated into two parts

$$\int_0^\infty = \int_0^\sigma + \int_\sigma^\infty .$$

For the first integral we obtain the upper bound

$$\int_0^\sigma e^{-\tau} \| V_{\tau/\varepsilon}^* U_{\tau/\varepsilon} f - f_- \| \, d\tau \leqslant \sigma (\| f \| + \| f_- \|)$$

We then choose $\delta > 0$ and arbitrary, determine a

$$\sigma \leqslant \frac{1}{2} \frac{\delta}{\| f \| + \| f_- \|} ,$$

and then an ε such that for all $t > \sigma/\varepsilon$

this gives

$$\| V_t^* U_t f - f_- \| < \frac{1}{2} \delta$$

$$\int_0^\infty e^{-\tau} \| V_{\tau/\varepsilon}^* U_{\tau/\varepsilon} f - f_- \| \, d\tau < \frac{1}{2} \frac{\delta}{\| f \| + \| f_- \|} (\| f \| + \| f_- \|)$$

$$+ \frac{1}{2} \delta \int_0^\infty e^{-\tau} d\tau = \delta .$$

Therefore the limit

$$\lim_{\varepsilon \to +0} \varepsilon \int_0^\infty e^{-\varepsilon t} V_t^* U_t f$$

exists and is equal to f_-, q.e.d. Since the limit which occurs in the bypothesis of lemma 6 is assumed to exist throughout $\mathfrak{H}$ [property (I)], we have established the existence of $\lim_{\varepsilon \to +0} \Omega_\varepsilon$ throughout $\mathfrak{H}$ also. This result is equally valid for the plus and minus case. We define

$$\Omega_\pm = \lim_{\varepsilon \to +0} \Omega_{\pm \varepsilon} . \tag{4.16}$$

We now assert that the adjoint operator $\Omega_\pm^*$ can be defined similarly as

$$\Omega_\pm^* = \lim_{\varepsilon \to +0} \Omega_{\pm \varepsilon}^* . \tag{4.17}$$

This is not a trivial consequence of (4.16) as might be inferred. Indeed the existence of the limit in (4.17) follows from lemma 6 only if the limit of

the integrand exists for $t \to \pm \infty$. However for states $f \varepsilon Q = R^{\perp}$ this limit of the integrand does not exist. Hence lemma 6 cannot be applied. It is however true that (4.16) implies the existence of the weak limit in (4.17). The assertion (4.17) is meant to be the strong limit and needs a separate proof.

For states $f \varepsilon R$ the limit does exist since for such states lemma 6 is applicable. Thus we need only to show the existence of the limit in case $f \varepsilon Q = R^{\perp}$. Because of our condition (III) $f \varepsilon Q$ implies $f \varepsilon M$ where M is the subspace spanned by the proper elements of H. Let $\varphi_1, \varphi_2, \ldots$ be a complete finite or infinite orthonormal system of elements in M such that

$$f = \sum_{\alpha} c_{\alpha} \varphi_{\alpha} \qquad (\sum | c_{\alpha} |^2 < \infty).$$

We can choose the φ_{α} in such a way that

$$H \varphi_{\alpha} = \omega_{\alpha} \varphi_{\alpha},$$

where ω_{α} are the proper values of H which may not all be different from each other. We have then

$$V_t f = \sum_{\alpha} c_{\alpha} e^{i \omega_{\alpha} t} \varphi_{\alpha}$$

and

$$\Omega_{\varepsilon}^{*} f = \varepsilon \int_0^{\infty} e^{-\varepsilon t} U_t^{*} V_t f \, dt = \int_0^{\infty} \sum e^{-(\varepsilon + i \omega_{\alpha}) t} U_t^{*} c_{\alpha} \varphi_{\alpha} \, dt = i \varepsilon \sum R_{\lambda_{\alpha}} C_{\alpha} \varphi_{\alpha}.$$

In this last expression we have introduced the *Resolvent* operators associated with H_0

$$R_{\lambda_{\alpha}} = -i \int_0^{\infty} e^{(\varepsilon + i \omega_{\alpha}) t} U_t^{*} \, dt = (H_0 - \lambda_{\alpha})^{-1}. \quad \lambda_{\alpha} = \omega_{\alpha} - i \varepsilon.$$

These operators are bounded linear operators for all values of λ different from the spectrum and therefore for all $\varepsilon > 0$. We shall now prove the

Lemma 7: If H_0 has no point spectrum then $\lim_{\varepsilon \to +0} \varepsilon R_{\lambda_{\alpha}} \varphi_{\alpha} = 0$ for all α.

Proof: Let λ be any of the λ_{α} and $\omega = \omega_{\alpha}$ the corresponding eigenvalue and $\varphi = \varphi_{\alpha}$ the corresponding eigenfunction of H

$$\varepsilon^2 \| R_{\lambda} \varphi \|^2 = \varepsilon^2 (R_{\lambda} \varphi, R_{\lambda} \varphi) = \varepsilon^2 (\varphi, R_{\lambda}^{*} R_{\lambda} \varphi).$$

The right-hand side can be transformed by using $R_{\lambda}^{*} = R_{\lambda^*}$ and the Hilbert relation valid for any pair λ, μ:

$$R_{\mu} - R_{\lambda} = (\mu - \lambda) R_{\mu} R_{\lambda}.$$

We then obtain

$$\varepsilon^2 \| R_{\lambda} \varphi \|^2 = \frac{\varepsilon^2}{\lambda^* - \lambda} (\varphi, (R_{\lambda^*} - R_{\lambda}) \varphi).$$

We now use the spectral decomposition of R_λ and after a slight rearrangement of the integrand arrive at the expression

$$\varepsilon^2 \| R\varphi \|^2 = \int_{-\infty}^{+\infty} \frac{\varepsilon^2}{(\varrho-\omega)^2+\varepsilon^2}\, d\big(\varphi, E(\varrho)\varphi\big) = \int_{-\infty}^{+\infty} \frac{\varepsilon^2}{\sigma^2+\varepsilon^2}\, d\big(\varphi, E(\omega+\sigma)\varphi\big) .$$

The integral has a positive integrand and a non-decreasing expression after the d-sign hence we can obtain an upper bound for it by separating the integral into three parts as follows:

$$\int_{-\infty}^{+\infty} = \int_{-\infty}^{-\eta} + \int_{-\eta}^{+\eta} + \int_{+\eta}^{+\infty} \qquad (\eta > 0) .$$

For the second part we replace the integrand by

$$1 \geqslant \frac{\varepsilon^2}{\varrho^2+\varepsilon^2}$$

in the other two by

$$\frac{\varepsilon^2}{\eta^2+\varepsilon^2} \leqslant \frac{\varepsilon^2}{\varrho^2+\varepsilon^2} .$$

and then replace the sum of the first and third by an integral from $-\infty$ to $+\infty$. In this manner we obtain

$$\varepsilon^2 \| R_\lambda \varphi \|^2 \leqslant \int_{-\eta}^{+\eta} d\left(\varphi, E(\omega+\sigma)\varphi\right) + \frac{\varepsilon^2}{\eta^2+\varepsilon^2} \int_{-\infty}^{+\infty} d\left(\varphi, E(\omega+\sigma)\varphi\right) .$$

$$= \left(\varphi, E(\omega+\eta)\varphi\right) - \left(\varphi, E(\omega-\eta)\varphi\right) + \frac{\varepsilon^2}{\eta^2+\varepsilon^2} .$$

In the limit $\varepsilon \to +0$ the last term vanishes, and since η was arbitrary we finally have

$$\lim_{\varepsilon \to +0} \varepsilon^2 \| R_\lambda \varphi \|^2 \leqslant \left(\varphi, \left[E(\omega+0) - E(\omega-0)\right]\varphi\right).$$

Since H_0 has no point spectrum the right-hand side is zero, consequently

$$\lim_{\varepsilon \to +0} \varepsilon \| R_\lambda \varphi \| = 0$$

or

$$\lim_{\varepsilon \to +0} \varepsilon\, R_\lambda \varphi = 0 , \quad \text{q. e. d.}$$

It follows from this that

$$\lim_{\varepsilon \to +0} \Omega_\varepsilon^* f = 0 \quad \text{for} \quad f \in M .$$

We can now summarize the result of this section with the following

Theorem:

In a scattering system described by the self-adjoint energy operators H and H_0 and the corresponding unitary operators

$$V_t = e^{-iHt},\ U_t = e^{-iH_0 t}$$

the operators

$$\Omega_- = \lim_{\varepsilon \to +0} \varepsilon \int_0^\infty e^{-\varepsilon t} V_t^* U_t$$

and

$$\Omega_-^* = \lim_{\varepsilon \to +0} \varepsilon \int_0^\infty e^{-\varepsilon t} U_t^* V_t$$

exist throughout the underlying Hilbert space $\mathfrak{H}$ and they are boundet linear operators with upper bound 1. They satisfy the relations

$$\Omega_-^* \Omega_- = I\ ,\quad \Omega_- \Omega_-^* = 1 - E_M\ ,$$

where E_M is the projection into the subspace of bound states.

A similar result holds for the operators

$$\Omega_+ = \lim_{\varepsilon \to +0} \varepsilon \int_{-\infty}^0 e^{\varepsilon t} V_t^* U_t$$

$$\Omega_+^* = \lim_{\varepsilon \to +0} \varepsilon \int_{-\infty}^0 e^{\varepsilon t} U_t^* V_t .$$

We conclude this section with the remark that the particular type of averaging which is used in the integral representation of $\Omega_\pm$ and $\Omega_\pm^*$ is not essential. Indeed it is possible to obtain the same operators in the form of a limit $\Omega_- = \lim_{T \to \infty} \Omega_{-T}$, where for instance

$$\Omega_{-T} = \frac{1}{T} \int_0^T V_t^* U_t \, dt .$$

The existence of this limit can be proved with similar methods and it can be shown that the result is identical with the result obtained with the other process.

In this form the result appears as a generalization of the so-called mean ergodic theorem of VON NEUMANN[14]).

The theorem is proved here only under the rather restrictive assumptions of the scattering systems. It is an interesting but unsolved problem wheather this generalized theorem is true for arbitrary continuous representations of the group of real numbers. As we shall see in the next section, if it were possible to assert this, one could formulate necessary *and* sufficient conditions for a system to be a scattering system.

5. Properties of Scattering Systems

We have already shown in Section 3 that the wave operators are linear isometries with the property

$$\Omega_-^* \Omega_- = \Omega_+^* \Omega_+ = I$$

$$\Omega_- \Omega_-^* = \Omega_+ \Omega_+^* = I - E_M$$

where E_M is the projection into the subspace of proper elements of H. We shall now use the integral representation of the preceding section to derive some further properties of this operator. The first of these is contained in the

Theorem:

The operators Ω are intertwining operators for the representations U_t and V_t:

$$\Omega\, U_t = V_t \Omega. \tag{5.1}$$

Proof:

We shall prove the theorem for $\Omega = \Omega_-$ only, in the other case the proof is similar and need not be given.

$$\Omega_\varepsilon\, U_s = \varepsilon \int_0^\infty e^{-\varepsilon t}\, V_t^*\, U_t\, U_s\, dt = \varepsilon \int_0^\infty e^{-\varepsilon t}\, V_t^*\, U_{t+s}\, dt$$

$$= \varepsilon\, V_s \int_s^\infty e^{-\varepsilon t \cdots + \varepsilon s}\, V_t^*\, U_t\, dt.$$

Hence

$$\Omega_\varepsilon\, U_t = V_t \Omega_\varepsilon + \varepsilon X,$$

where X is some bounded operator for all $\varepsilon \geqslant 0$. Since the limit $\varepsilon \to +0$ exists everywhere in $\mathfrak{H}$ we obtain for $\varepsilon \to +0$ Eq. (5.1), q.e.d.

By taking the adjoint operators in (5.1) we obtain the

Corollary:

The operators Ω^* satisfy

$$\Omega^*\, V_t = U_t \Omega^*. \tag{5.2}$$

There are several interesting consequences which follow from this theorem and its corollary.

Define the one-parameter operator family

$$\Omega(t) = U_t^* \, \Omega \, U_t . \tag{5.3}$$

Then we have the

Theorem:

The lim $\Omega(t)$ exists and we have

$$\lim_{t \to -\infty} \Omega_+(t) = \lim_{t \to +\infty} \Omega_-(t) = I \tag{5.4}$$

$$\lim_{t \to +\infty} \Omega_+(t) = S \tag{5.5}$$

$$\lim_{t \to -\infty} \Omega_-(t) = S^{-1}. \tag{5.6}$$

Proof:

By using (5.1) we have $\Omega(t) = U_t^* \, V_t \, \Omega$. The operator limit $U_t^* \, V_t$ exists on the range R of Ω [Eq. (3.7)] and is there equal to Ω^* for $t \to \pm\infty$. Hence

$$\lim_{t \to -\infty} \Omega_+(t) = \Omega_+^* \, \Omega_+ = I$$

$$\lim_{t \to +\infty} \Omega_-(t) = \Omega_-^* \, \Omega_- = I$$

$$\lim_{t \to +\infty} \Omega_+(t) = \Omega_-^* \, \Omega_+ = S$$

$$\lim_{t \to -\infty} \Omega_-(t) = \Omega_+^* \, \Omega_- = S^{-1}.$$

This result leads to a new and equivalent definition of the scattering operator S through Eq. (5.5) or (5.6).

Since these limits exist everywhere in $\mathfrak{H}$, the operator

$$\Omega(t) \, \Omega^*(t) = 1 - E_M(t)$$

with

$$E_M(t) = U_t^* \, E_M \, U_t$$

also has limits for $t \to \pm \infty$ and because of (5.4)

$$\lim_{t \to \pm \infty} E_M(t) = 0. \tag{5.7}$$

With the results so far obtained we can now clear up a paradox which has often been discussed in the literature but which has never been completely understood. The paradox appears when one discusses the family of transformation operators

$$U(t, t_0) \equiv U_t^* \, V_t \, V_{t_0}^* \, U_{t_0}.$$

This is a two-parameter family of unitary operators, with the properties

$$U(t, t_0) = U^* (t_0, t) \tag{5.8}$$

$$U(t_0, t_0) = I , \tag{5.9}$$

$$U(t_1, t)\ U(t, t_0) = U(t_1, t_0) \tag{5.10}$$

Such an operator family is obtained if one 'solves' formally the Schrödinger equation in the interaction picture

$$i \frac{\partial t}{\partial} U(t, t_0) = V(t)\ U(t, t_0) \tag{5.11}$$

with the 'initial condition' (5.9). The same equation is satisfied by te operators $\Omega_+(t)$

$$i \frac{\partial}{\upsilon t} \Omega_+(t) = V\ (t)\, \Omega_+\ (t) \tag{5.12}$$

and they satisfy the 'initial condition'

$$\Omega\ (-\infty) = I$$

Hence one would expect to have

$$\Omega\ (t) = U\ (t, -\infty) \tag{5.13}$$

if the implied limit on the right exists. The paradox comes from the fact that $U(t_1\ t_0)$ is unitary for *all* t_0 while $\Omega(t)$ is not, in fact

$$\Omega\ (t)\, \Omega^*\ (t) = I - E_M\ (t)$$

The obvious answer, which occasionally has been given, that the limit $U(t, t_0)$ for $t_0 \to -\infty$ does not exist if H has discrete eigenvalues, is incorrect. Indeed the operator $V^*_{t_0} U_{t_0}$ does have a limit for $t_0 \to -\infty$ on all of $\mathfrak{H}$ (condition I) and the equation (5.13) is a correct equation as one can easily verify with the help of the relations (5.1) and (5.2). The solution of the paradox lies in the observation that the limit $U^*(t, t_0)$ for $t_0 \to -\infty$ does not exist on all of $\mathfrak{H}$, because the operator $U^*_{t_0} V_{t_0}$ has no limit for vectors with non-vanishing components in M. Without the existence of this limit the unitary property of $U(t, t_0)$ is destroyed for $t_0 \to -\infty$. Hence the paradox is resolved.

Among the more interesting consequences of the intertwining property of the wave operators are those which follow from the application of Schur's lemma. This lemma can be formulated as follows: Let Q be the nul-space of Ω, that is the set of vectors $f \varepsilon \mathfrak{H}$ such that $\Omega f = 0$ and R the closure of the range of Ω, and Q^*, R^* the corresponding quantities for Ω^*. These are all subspaces of $\mathfrak{H}$, and $R^\perp = Q^*$, $Q^\perp = R^*$. Schur's lemma

then says: R is an invariant subspace for V_t and R^* is an invariant subspace for U_t and the reduction of V_t to R is unitarily equivalent to the reduction of U_t to R^*:

$$^{R}V_t \simeq {}^{R^*}U_t.$$

In our particular case $R^* = Q^{\perp}$ is the whole space $\mathfrak{H}$ since R^* is equal to the domain of definition of Ω (condition I). Hence for scattering systems:

$$^{R}V_t \simeq U_t. \tag{5.14}$$

Since $R = Q^{*\perp} = M^{\perp}$ is the subspace of the continuum states of H we can express (5.14) in the following manner:

The operator U_t is unitarily equivalent to the reduction of V_t to the continuum states of H.

As a corollary we have: The continuous parts of the spectra for H and H_0 are identical.

We have here found a necessary condition for a system characterized by H and H_0 to be a scattering system. It is an interesting question whether this condition is also sufficient. It can be shown that the answer would be yes if it were possible to establish a generalized mean ergodic theorem (section 4) for unitarily equivalent representations U_t and V_t. However we have not been able to do this and the question must be left open for the time being.

We shall now establish a few additional properties of bounded linear operators Ω, with the intertwining property

$$\left.\begin{aligned} \Omega_1 U_t &= V_t \Omega_1 \\ \Omega_1^* V_t &= U_t \Omega_1^*. \end{aligned}\right\} \tag{5.15}$$

The study of such general operators will give us a third definition of the scattering operator S.

Let R_1 be the closure of the range of Ω and R_1^* the closure of the range of Ω_1^*. These are subspaces of $\mathfrak{H}$. Schur's lemma gives

$$^{R_1}V_t \simeq {}^{R_1^*}U_t. \tag{5.16}$$

Let R denote as before the common range of Ω_+ and Ω_- (property II). Then we have the

Lemma 1: The range of R_1 of Ω_1 is contained in the range R of Ω: $R_1 \subset R$.

Proof: Since $R_1^* \subset \mathfrak{H}$ the representation $^{R_1^*}U_t$ is contained in U_t. We use for this relation the notation

$$^{R_1^*}U_t \lesssim U_t.$$

By applying Schur's lemma twice we obtain the equivalence relations

$$ {}^{R_1}V_t \simeq {}^{R_1*}U_t \lesssim U_t \simeq {}^{R}V_t . $$

Hence

$$ {}^{R_1}V_t \lesssim {}^{R}V_t . $$

This means*)

$$ R_1 \mathbf{C} R \text{ , q. e. d.} $$

Lemma 2. For every intertwining operator Ω_1 of a scattering system the operator $\Omega_1(t) = U_t^* \Omega_1 U_t$ has limits at $t \to \pm \infty$.

Proof: The intertwining property yields

$$ \Omega_1 (t) = U_t^* V_t \Omega_1 $$

and the limits $U_t^* V_t f$ for $t \to \pm \infty$ exist for $f \varepsilon R$. [See eq. (3.7)]. Every f of the form $f = \Omega_1 g$, is in R_1 and therefore by lemma 1 also in R. Thus $\lim_{\to +\infty} \Omega_1(t)\, g$ exists for all $g \varepsilon \mathfrak{H}$, q.e.d.

Lemma 3. Every intertwining operator Ω_1 determines uniquely two operators X_+ and X_- such that

$$ \Omega_1 = \Omega_+ X_+ = \Omega_- X_- $$

and X_+ and X_- commute with U_t.

Proof: We prove one case only and omit the sign index. Define

$$ \Omega^* \Omega_1 = X $$

then

$$ \Omega \Omega^* \Omega_1 = \Omega X = (1 - E_{Q^*}) \Omega_1 . $$

Now $Q^* = R^\perp$, and E_{Q^*} is the projection into the subspace $R^\perp$. By lemma 1 the range R_1 is contained in R and consequently all $f \varepsilon R_1$ are orthogonal to $Q^* = R^\perp$. This yields

$$ E_{Q^*} \Omega_1 = 0 $$

and

$$ \Omega X = \Omega_1 . $$

Furthermore the intertwining property for Ω and Ω_1 implies that X commutes with U_t, q.e.d.

Definition:

An intertwining operator Ω_1 is called *complete* if $R_1 = R$.

Lemma 4. An intertwining operator Ω_1 is complete if and only if the X of lemma 3 has an inverse.

---

*) *Note added in proof:* This conclusion does not follow from the preceding equation. A corrected proof of this lemma will be given elsewhere.

Proof: Assume Ω_1 is complete. Denote by $\Omega^*(R_1)$ the subspace of vectors of the form $\Omega^* f$ with $f \varepsilon R_1$. The operator X maps $\mathfrak{H}$ onto the subspace $\Omega^*(R_1)$. But if Ω_1 is complete $R_1 = R$ and $\mathfrak{H}^*(R_1) = \mathfrak{H}$. Thus the range of X is $\mathfrak{H}$. We next show that $f \neq 0$ implies $g = X f \neq 0$. If $g = 0$ then $\Omega_1 f \varepsilon Q^* = R^{\pm}$, but $\Omega_1 f \varepsilon R_1 = R$, therefore $\Omega_1 f = 0$, or $f \varepsilon Q_1 = R^{*\pm}$. Now for a scattering system $R^* = \mathfrak{H}$. Hence $R^{*\pm} = R_1^{*\pm} = Q_1 = 0$ and therefore $f = 0$. Thus we have shown X has an inverse for every $f \varepsilon \mathfrak{H}$, q.e.d. Conversely if X has an inverse, we can write $\Omega = \mathfrak{H}_1 X^{-1}$. Therefore if $f \varepsilon R$ then $f = \Omega g$ for some $g \varepsilon \mathfrak{H}$ and consequently $f = \Omega_1 X^{-1} g$. This means $f \varepsilon R_1$ and $R \mathbf{C} R_1$. But by lemma 1 $R_1 \mathbf{C} R$ and we conclude $R = R_1$, q.e.d.

Corollary: If Ω_1 and Ω_2 are two complete intertwining operators then there exists a linear operator Z such

$$\Omega_1 = \Omega_2 Z \tag{5.17}$$

and

$$[Z, U_t] = 0 .$$

If

$$\Omega_1 = \Omega X_1 \text{ and } \Omega_2 = \Omega X_2$$

then

$$Z = X_2^{-1} X_1 .$$

In the case that Ω_1 and Ω_2 are the operators Ω_+ and Ω_- respectively the operator Z of the corollary is simply the S-operator. The commuting property of S with U_t is the mathematical expression for the law of the conservation of energy.

Theorem: Let U_t and V_t be the unitary representations of the additive group of real numbers associated with a scattering system and Ω_1 any complete intertwining operator, then the limits of the operator family $\Omega_1(t) = U_t^* \Omega_1 U_t$ exist for $t \to \pm \infty$ and

$$\Omega_1 (+ \infty) = S \Omega_1 (- \infty) \tag{5.18}$$

where S is the scattering operator:

Proof: Existence of the limits is assured by lemma 2. According to lemma 3 there exists a unique bounded linear operator X, such that

$$\Omega_1 = \Omega_+ X .$$

Since X commutes with U_t, we also have

$$\Omega_1 (t) = \Omega_+ (t) X$$

and consequently

$$\Omega_1 (- \infty) = \Omega_+ (- \infty) X = X$$

$$\Omega_1 (+ \infty) = \Omega_+ (+ \infty) X = S X .$$

Combining the last two equations, we find

$$\Omega_1 (+\infty) = S\,\Omega_1 (-\infty)$$

which proves the theorem.

The content of this theorem can be used for a new definition of the scattering operator S: Given U_t, V_t of a scattering system, find a complete intertwining operator Ω_1 and then define S by (5.18).

6. The Scattering Cross Section

In the preceding sections we have established that the so-called 'simple scattering systems' characterized by the properties (I), (II), and (III) always admit a unitary scattering operator. It is not immediately obvious how this operator is related to the physically observable quantities in a scattering process. These quantities are always expressed in terms of the *scattering cross-section*. Hence our problem is to show how the scattering cross section is obtained from the unitary scattering operator.

The formal procedure for calculating the scattering cross section is well known*). We shall derive this result here from a mathematically more satisfactory point of view. All derivations of the cross section which have been given either make use of improper function or artificial devices such as normalized wave functions in a box which are entirely foreign to the physical problem on hand. It may, therefore, be not superfluous to show how the cross section can be obtained without any artificial devices of this nature. In the derivation here presented we shall at all stages stay very close to the actual physical situation.

Before we do this we must first examine an assumption which is always made as a matter of course viz. that every S-operator can be represented as an S-matrix. It is well-known that the association of an integral operator with a unitary operator is not always possible. The simplest example is the unit operator. Hence we must first examine in what sense it is possible to associate an integral operator with the S-operator.

In order to make the discussion specific we shall examine the simplest case, viz. the scattering of a single particle with no internal degrees of freedom. The interaction is then necessarily an external one, such that the total momentum of the particle is changed in the scattering process. The case of the scattering of two particles is easily reduced to this case, for instance, by separating the center of mass motion from that of the relative motion. It is equally simple to include internal degrees of freedom.

*) See for instance reference 1 esp. chapt. 8.

In order to study the matrix-representation of the S-operator we shall introduce a relaziation of the Hilbert space by the family of L^2-functions $f(\boldsymbol{k})$ over the infinite domain of the three-dimensional Euclidean space. It is well-known that in such a realization the three-momentum operators p_i can be written as multiplication with k_i, and that this realization is essentially (that is apart from unitary equivalence) unique[15]).

In this realization the operator H_0 is given by

$$H_0 f(\boldsymbol{k}) = \omega(k) f(\boldsymbol{k}) \tag{6.2}$$

where

$$\omega(k) \quad \text{either} \quad \frac{1}{2m} k^2 \quad \text{or} \quad \sqrt{k^2 + m^2}.$$

In any case $\omega(k)$ is a monotonically increasing function of k, such that

$$\omega(k) < \omega(k') \quad \text{for} \quad k < k'$$

If S has a representation as an integral operator then there exists a function $S(\boldsymbol{k}, \boldsymbol{k}')$ of the six variables $\boldsymbol{k}$ and $\boldsymbol{k}'$ such that

$$S f(\boldsymbol{k}) = \int S(\boldsymbol{k}, \boldsymbol{k}') f(\boldsymbol{k}') \, d^3 k'. \tag{6.3}$$

It is easy to show that for the S-operators such a representation can never exist. This is a simple consequence of the fact that S commutes with H_0, that is, the equation

$$S H_0 f = H_0 S f \tag{6.4}$$

holds for all $f \varepsilon D_{H_0}$. When this equation is expressed in terms of the functions $f(\boldsymbol{k})$ there results

$$\int S(\boldsymbol{k}, \boldsymbol{k}') \left(\omega(k) - \omega(k')\right) f(\boldsymbol{k}') \, d^3 k' = 0. \tag{6.5}$$

This equation holds for all $f(\boldsymbol{k})$ such that

$$\int \omega^2(k) \, | f(\boldsymbol{k}) |^2 \, d^3 k < \infty$$

The set of vectors with this property is everywhere dense and from this one concludes by a well-known reasoning that almost everywhere

$$S(\boldsymbol{k}, \boldsymbol{k}') \left(\omega(k) - \omega(k')\right) = 0 \tag{6.6}$$

and also

$$S(\boldsymbol{k}, \boldsymbol{k}') = 0 \quad \text{for} \quad k \neq k'. \tag{6.7}$$

Since the surface $\omega(k) =$ const. has measure zero with respect to the volume integration we find

$$\int S^*(\boldsymbol{k}, \boldsymbol{k}'') \, S(\boldsymbol{k}', \boldsymbol{k}'') \, d^3 k'' = 0$$

which is incompatible with the unitary property of S. Hence the representation (6.3) does not exist.

We have here of course merely expressed the well-known fact that 'the S-matrix must contain a δ-function with respect to the energy'.

Even though a matrix representation of S is seen not to exist, it is possible that there might exist a matrix representation in the following sense: Introduce spherical polarcoordinates in $\boldsymbol{k}$-space and denote a point on the unit sphere with α and the corresponding (two-dimensional) surface element with $d\alpha$. Writing $f(k, \alpha)$ for the functions in L^2 we may find a function $R_{\alpha\alpha'}(k)$ of the pairs α, α' such that

$$S f(k, \alpha) = f(k, \alpha) + \int R_{\alpha\alpha'}, (k) f(k, \alpha') d\alpha' . \tag{6.8}$$

An interpretation of scattering in terms of a differential cross section is only possible in terms of the matrix elements $R_{\alpha\alpha'}$. Hence the existence of such a matrix is a necessary requirement for this interpretation. We shall, therefore, make the assumption that (6.8) exists and proceed to show how the cross section is defined in terms of the matrix elements $R_{\alpha\alpha'}$.

We simplify the notation by suppressing the parameter k on which all quantities depend. In the physical interpretation of quantum mechanics

$$P(\alpha) \equiv \int\int R^*_{\alpha\alpha'}, R_{\alpha\alpha''} f^*(\alpha') f(\alpha'') d\alpha' d\alpha'' \tag{6.9}$$

represents the probability density for the observation of a scattered particle with the propagation direction α. In this form the result is not yet susceptible to a physical interpretation. The reason is, that scattering experiments are not performed with a single scatterer but with a target which contains a large number of independent scatterers at different locations in space. What is observed then is not the probability density (6.9) but an average of this quantity over a large number of scatterers in the target.

There are two conditions which a good target should satisfy. The first is that it must not be too thick so that multiple scattering inside the target is negligeable. The second is, that the scatterers in the target should be arranged in an essentially random manner so that there are no phase relations of the scattered waves arriving from different scattering centers. These two conditions allow us to calculate the average value of the probability $P(\alpha)$ by summing the contribution of the single scattering probability (6.9) from each individual scatterer in the target.

The S-operator $S(\boldsymbol{a})$ associated with a scatterer at the position $\boldsymbol{a}$ is obtained from the operator S of a scatterer at the origin by a similarity transformation

$$S(\boldsymbol{a}) = \Pi(\boldsymbol{a}) S \Pi^*(\boldsymbol{a}) \tag{6.10}$$

with the unitary displacement operator $\Pi(\boldsymbol{a})$ defined by

$$\Pi(\boldsymbol{a}) f(\boldsymbol{k}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{a}} f(\boldsymbol{k}) \tag{6.11}$$

From this we find for the corresponding matrix elements

$$R_{\alpha\alpha'}(\boldsymbol{a}) = e^{i\,\boldsymbol{a}\cdot(\boldsymbol{k}'-\boldsymbol{k})}\, R_{\alpha\alpha'} \tag{6.12}$$

with

$$k = k'\,.$$

We shall now make the assumption that the number of scatterers in the target is so large that one may, with sufficient accuracy, calculate the average scattering probability by replacing the sum over the individual scatterers by an integral. When this is done we arrive at the following expression for the average probability density $\overline{P}(\alpha)$

$$\overline{P}(\alpha) = n\int d^3a \int\int d\alpha'\, d\alpha''\, e^{i(\boldsymbol{k}'-\boldsymbol{k}'')\cdot\boldsymbol{a}}\, R^*_{\alpha\alpha'}\, R_{\alpha\alpha''}\, f^*(\alpha')\, f(\alpha'')\,. \tag{6.13}$$
$$(k' = k'' = k)$$

where $n\,d^3a$ is the (constant) number of scatterers inside the volume element d^3a and the integral d^3a is to be carried out over the entire target volume.

In order to evaluate this integral we adapt the coordinate system to the geometrical configuration of the target. Let the 3-component of $\boldsymbol{a}$ be normal to the target area and the 1- and 2-components in the target area which is assumed to extend in all directions without limit. The integral over a_1 and a_2 can then be evaluated with the Fourier integral theorem. We keep α'' fixed, define $\boldsymbol{g} = \boldsymbol{k}' - \boldsymbol{k}''$, introduce spherical coordinates ϑ, φ such that

$$d\alpha' = \sin\vartheta\, d\vartheta\, d\varphi\,.$$

If the polar axis is in the direction of g_3 we have

$$g_1 = k\sin\vartheta\cos\varphi$$

$$g_2 = k\sin\vartheta\sin\varphi$$

$$g_3 = k(\cos\vartheta - 1)$$

so that

$$d\alpha' = \frac{\partial(\vartheta,\varphi)}{\partial(g_1, g_2)}\, dg_1\, dg_2 = \frac{dg_1\, dg_2}{k\sqrt{k^2 - g_1^2 - g_2^2}}\,.$$

The resulting integral is of the form

$$\int da_1\, da_2 \int e^{i(g_1 a_1 + g_2 a_2)}\, F(g_1\, g_2)\, dg_1\, dg_2 = (2\pi)^2\, F(0,0)\,, \tag{6.14}$$

where

$$F(g_1\, g_2) = n\,\frac{1}{k\sqrt{k^2 - g_1^2 - g_2^2}}\, R^*_{\alpha\alpha'}\, R_{\alpha\alpha''}\, f^*(\alpha')\, f(\alpha'')\,.$$

The remaining integration over a_3 is now trivial, since the integrand which

is left after the substitution (6.14) is independent of a_3. Denoting by d the thickness of the target we arrive at the final result:

$$\overline{P}(\alpha) = (2\pi)^2 n d \int d\alpha' \frac{1}{k^2} |R_{\alpha\alpha'}|^2 |f(\alpha')|^2 . \tag{6.15}$$

The quantity

$$\sigma = \frac{(2\pi)^2}{k^2} |R_{\alpha\alpha'}|^2 , \tag{6.16}$$

which has the dimension of an area, is the differential scattering cross section for the scattering of a particle with direction α' into a particle with direction α.

It is easily seen that formulae (6.15) and (6.16) correspond exactly to the usual description of the scattering process in terms of the cross section. Indeed, if the direction of the incident particles is equal to α_0 to a very high degree of approximation then this situation would be described by a wave packet $f(\alpha')$ with a sharply peaked probability amplitude around $\alpha' = \alpha_0$. In this case the probability density for scattering into the direction α would be described with a high degree of accuracy

$$\overline{P}(\alpha) = n \cdot d \cdot \sigma . \tag{6.17}$$

This is the usual expression of this quantity in terms of the cross section σ.

7. Concluding remarks

In the preceding sections we have given three equivalent definitions of the scattering operator and we have proved the existence of this operator for simple scattering systems as well as its unitary property.

With this result we have succeeded to place the theory of scattering processes on a rigorous mathematical foundation. The results obtained here, as well as the new methods introduced, may be the incentive for a number of further investigations. Foremost among these is the general scattering formalism for the multichannel processes and the investigation of the scattering operator in field theories.

The author has received considerable help from Professor H. A. DYE of the University of Southern California who pointed out to him the connection with the Mean Ergodic Theorem, and from Professor G. W. MACKEY of Harvard University for an interesting suggestion and a counter example. Several conversations with my colleagues, Professor M. SMILEY and Professor S. K. BERBERIAN of this University have been very helpful. To all of them I wish to express here my thanks.

References

[1]) J. M. JAUCH and F. ROHRLICH, 'Theory of Photons and Electrons', Addison-Wesley Publishing Co. (1955), esp. Chap. 7.

[2]) T. IMAMURA, Progr. of Theor. Phys. *18*, 51 (1957)

[3]) H. E. MOSES, Nuovo Cim. *1*, 103 (1955).

[4]) F. COESTER, M. HAMMERMESH, and K. TANAKA, Phys. Rev. *96*, 1142 (1954).

[5]) M. N. HACK, Phys. Rev. *96*, 196 (1954)

[6]) F. J. BELINFANTE and C. MOLLER, Kgl. Danske Vid. Selskab, Mat.-fys. Medd. 28, No. 6 (1953)

[7]) S. T. MA, Phys. Rev. *87*, 652 (1952).

[8]) M. GELL-MANN and M. GOLDBERGER, Phys. Rev. *91*, 398 (1953).

[9]) S. FUBINI, Atti, Acad. Naz. Lincei *12*, 298 (1952).

[10]) H. EKSTEIN, Phys. Rev. *101*, 880 (1956); *94*, 1063 (1954).
A review of the 'formal' theory of scattering is found in B. S. DE WITT, 'The Operator Formalism in Quantum Perturbation Theory', University of California, Radiation Laboratory. In this reference is also a complete list of the earlier publications on the scattering operator.

[11]) J. VON HEUMANN, «Mathematische Grundlagen der Quantenmechanik», J. Springer, Berlin, 1932.

[12]) E. L. HILL, Phys. Rev. *104*, 1173 (1956); *107*, 877 (1957).

[13]) The material in this section can be found in a large number of references. For the the convenience of the reader we mention only the following which we have found most useful. – J. VON NEUMANN, «Mathematische Grundlagen der Quantenmechanik», J. Springer, Berlin 1932. – F. RIESZ and B. SZ.-NAGY, 'Functional Analysis', F. Ungar Publ. Co., New York 1955. – M. H. STONE, 'Linear Transformations in Hilbert Space», Am. Math. Soc. Coll. Publ. XV, New York 1932. – N. I. ACHIESER and I. M. GLASMANN, 'Theorie der linearen Operatoren im Hilbert Raum', Akademie Verlag, Berlin 1954.

[14]) J. VON NEUMANN, Proc. Nat. Acad. *18*, 70 (1932).

[15]) J, VON NEUMANN, Math. Ann. *104*, 570 (1931).