Van Nieuwenhuizen, P.
Ruijgrok, Th.
1967

Physica 33
595-606

THE S-MATRIX FOR SCATTERING OF COMPOSITE SYSTEMS

by P. VAN NIEUWENHUIZEN and TH. RUIJGROK

Instituut voor theoretische fysica der rijksuniversiteit, Utrecht, Nederland

Synopsis

It is shown that the asymptotically stationary states, as introduced by Van Hove[1]), provide a natural tool to describe the scattering of composite systems. The scattering problem is formulated in terms of these a.s. states and a unitary S-matrix is defined. In this paper we treat the formal aspects with complete mathematical rigour. The method can be used to derive an alternative form of the Faddeev equations[2])[3]).

1. *Introduction.* A much discussed problem in quantum mechanics is the question of how the S-matrix should be defined for scattering by bound states. Because of the overlap of final states which then always takes place, this is a non-trivial problem. A different but related problem is the following. For the scattering of a particle by a bound state of other particles, the kernel of the "Lippman-Schwinger" equation for the resolvent $R(z)$ is not of Hilbert-Schmidt type and gives not even a completely continuous operator. The methods which are commonly used for the solution of the equations for two-body problems therefore do not apply. Faddeev, however, has shown that it is possible to formulate the equations for the scattering states in such a way that only (coupled) integral equations with completely continuous operators occur[2]). He considers two-body interactions by potentials whose Fourier transforms have certain, not very restrictive, properties. The actual calculation of the S-matrix, however, is very complicated. It is the purpose of the present paper to describe a method which is well suited for the description of scattering by bound states. With this method the definition of the S-matrix becomes a simple generalization of the well known case of two particle scattering. For its actual evaluation, the reduction method of Faddeev must be used again. This will be discussed in the following paper.

The fundamental idea is to span the Hilbert space by an overcomplete set of basic states $|\alpha\rangle$, which are formed by taking products of free particle states. A bound state of m particles is also considered as one free particle. The states $|\alpha\rangle$ have the property of being asymptotically orthonormal (a.o.) and asymptotically stationary (a.s.) These concepts are taken from van

Hove's work[1]) and will again be defined in section 2. If we now expand the stationary scattering states $|\alpha\rangle^{\pm}$ (solutions of the Schrödinger equation with definite boundary values) in terms of the a.s. states

$$|\alpha\rangle^{\pm} = |\alpha\rangle - \int \frac{c_{\beta\alpha}(\pm)}{\varepsilon_\beta - \varepsilon_\alpha \mp i0} |\beta\rangle \qquad (1)$$

the expansion coefficients $c_{\beta\alpha}(\pm)$ are not uniquely defined, due to the over-completeness (see section 2) of the a.s. states. It can be shown, however, (see section 4) that on the energyshell the $c_{\beta\alpha}(\pm)$ are unique. This implies that also the S-matrix, to be defined in section 3, is uniquely determined. In section 4 we will also show that our S-matrix is unitary.

A justification of the formal steps which will be taken in the following sections is given in an appendix. Although the results of this appendix are completely general we have given in section 5 a more detailed discussion of these formal steps for the case of three particle systems. The conclusions are collected in section 6. Before proceeding to the next section we want to make the following remark concerning the stationary states $|\alpha\rangle^{\pm}$ in (1). If the potentials describing the interactions between the particles are not invariant for translations the total momentum is not a conserved quantity and consequently there will be no restriction on the integration over β in (1). If, on the other hand, the total momentum is a constant of the motion we can take for $|\alpha\rangle$ states with a definite value $\boldsymbol{P}_\alpha$ of the total momentum and it will be understood that in the integration over β in (1) only those states $|\beta\rangle$ occur for which $\boldsymbol{P}_\beta = \boldsymbol{P}_\alpha$. Because $|\beta\rangle$ is a product state of n so called free particles this is easily realized by omitting from all quantum number β the ones giving the momentum of one free particle. The value of the latter is then determined by $\boldsymbol{P}_\beta = \boldsymbol{P}_\alpha$. A similar procedure is adopted when other conserved quantities (e.g. parity) exist.

2. *Asymptotically orthonormal and stationary states.* We assume that in one way or another a set of basic states $|\alpha\rangle$ is given which has the property that for any two square integrable functions $d_1(\alpha)$ and $d_2(\alpha)$ a (generalized) Fourier integral exists that maps in L^2 and that the wave packets

$$|\varphi_i(t)\rangle = \int d_i(\alpha)\, \mathrm{e}^{-i\varepsilon_\alpha t}\, |\alpha\rangle \qquad (i = 1, 2) \qquad (2)$$

satisfy

$$\lim_{t\to\pm\infty} \langle\varphi_i(t)|\varphi_j(t)\rangle = \int d_i^*(\alpha)\, d_j(\alpha) \qquad (i, j = 1, 2) \qquad (3)$$

(For an example of such integrals see section 5). The states $|\alpha\rangle$ will then be called asymptotically orthonormal.

In the case of a system of three different particles we take for the basic set $|\alpha\rangle$ the following states:

1. products of three plane waves: $|\alpha\rangle = |\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{k}_3\rangle$ with

$$\varepsilon_\alpha = \frac{\hbar^2 k_1^2}{2m_1} + \frac{\hbar^2 k_2^2}{2m_2} + \frac{\hbar^2 k_3^2}{2m_3}$$

2. the product of one free particle and a bound state of the other two; for example:

$$|\alpha\rangle = |\boldsymbol{k}_1; \boldsymbol{p}, n\rangle \quad \text{with} \quad \varepsilon_\alpha = \frac{\hbar^2 k_1^2}{2m_1} + \frac{\hbar^2 p^2}{2(m_2 + m_3)} - E(n),$$

where n chararacterizes the bound state of the two particles and $E(n)$ is its binding energy.

3. three particle bound states:

$$|\alpha\rangle = |\boldsymbol{p}, \tau\rangle \quad \text{with} \quad \varepsilon_\alpha = \frac{\hbar^2 p^2}{2(m_1 + m_2 + m_3)} - E(\tau),$$

where τ characterizes the bound state of the three particles and $E(\tau)$ is its binding energy.

In section 5 it will indeed be shown that these states are a.o. From this example it will be clear how in general we define states $|\alpha\rangle$ and the corresponding energies ε_α. It should be noted that, in order to construct these states for a system of n particles, all bound states of 2, 3, ..., $n - 1$ particles must be known. Furthermore we observe that, since the states of the type 1 by itself form a complete and orthonormal base, the set $|\alpha\rangle$ will in general be overcomplete. In this and the following paper we will be interested in scattering only and not in the case where all n particles are bound. For this reason we will omit the states of type 3 from our basic set, which remains overcomplete, however. The expansion coefficients $c_{\beta\alpha}(\pm)$ in the stationary scattering states (1) are therefore not uniquely defined. In spite of this fact it is nevertheless possible to use the scattering amplitudes for a unique definition of the S-matrix.

In a scattering experiment the observed initial and final states are precisely given by our asymptotic states $|\alpha\rangle$. The S-matrix must therefore be defined in terms of these states. Following Van Hove[1]) this is done as follows. Let $|\varphi(t)\rangle$ be a solution of the Schrödinger equation and let us suppose that coefficients $b(\alpha)$ and $\tilde{b}(\alpha)$ exist so that the norm of the state

$$|\varphi(t)\rangle - \int_\alpha \tilde{b}(\alpha)\, \mathrm{e}^{-i\varepsilon_\alpha t}\, |\alpha\rangle \quad \text{for} \quad t \to -\infty \tag{4}$$

and of the state

$$|\varphi(t)\rangle - \int_\alpha b(\alpha)\, \mathrm{e}^{-i\varepsilon_\alpha t}\, |\alpha\rangle \quad \text{for} \quad t \to +\infty \tag{5}$$

approaches zero. (Let $|\varphi(t)\rangle$ be orthogonal to the bound states)

If this property is satisfied for all solutions $|\varphi(t)\rangle$, the set of states $|\alpha\rangle$ will be called asymptotically stationary (a.s.).

3. *Definition of the S-matrix.* The S-matrix which is directly related to our experiment, is then defined by

$$\tilde{b}(\alpha) = \int_\beta S_{\alpha\beta} b(\beta). \tag{6}$$

In the remainder of this section we want to show that the coefficients $b(\alpha)$ and $\tilde{b}(\alpha)$ exist and are uniquely defined, and that there is no ambiguity in the definition of $S_{\alpha\beta}$. In section 4 the unitarity of S will be proved.

It is known that the solution $|\varphi(t)\rangle$ can be expanded uniquely in terms of the stationary scattering states $|\alpha\rangle^{\pm}$ as follows:

$$|\varphi(t) = \int_\alpha d_+(\alpha)\, \mathrm{e}^{-i\varepsilon_\alpha t}\, |\alpha\rangle^+ = \int_\alpha d_-(\alpha)\, \mathrm{e}^{-i\varepsilon_\alpha t}\, |\alpha\rangle^-. \tag{7}$$

This is the spectral decomposition theorem which can be applied since the Hamiltonian is always self-adjoint. For 3 particles Faddeev proved this spectral decomposition theorem (see ref. 3). Since we consider only scattering problems the energies ε_α are the same as the energies of the asymptotic states. $|\varphi(t)\rangle$ shall be normalized, so that

$$\langle\varphi(t)|\varphi(t)\rangle = \int d_\pm^*(\alpha)\, d_\pm(\alpha) = 1. \tag{8}$$

Consider now the states

$$|\psi_\pm(t)\rangle = \int d_\pm(\alpha)\, \mathrm{e}^{-i\varepsilon_\alpha t}\, |\alpha\rangle \tag{9}$$

with the same $d_\pm(\alpha)$ as in (2.7). In these states the scattering is not taken into account, so that $|\psi_\pm(t)\rangle$ is not a solution of the Schrödinger equation. In most cases the norm of these states will not be constant in time, because the basic states $|\alpha\rangle$ are not all orthogonal to each other. We have, however,

$$\lim_{t\to+\infty} \langle\psi_\pm(t)|\psi_\pm(t)\rangle = \lim_{t\to-\infty} \langle\psi_\pm(t)|\psi_\pm(t)\rangle = 1. \tag{10}$$

which follows from our assumption (3) that the states $|\alpha\rangle$ are asymptotically orthonormal.

Similarly we can show that for t $\to \mp\infty$ the norm of the state $|\varphi(t)\rangle - |\psi_\pm(t)\rangle$ tends to zero. We will prove this by showing that

$$\lim_{t\to\mp\infty} \langle\psi_\pm(t)|\varphi(t)\rangle = 1 \tag{11}$$

For that purpose we write $|\varphi(t)\rangle$ in the form

$$|\varphi(t)\rangle = \int_\alpha d_\pm(\alpha)\cdot \mathrm{e}^{-i\varepsilon_\alpha t}\, |\alpha\rangle - \int_\beta\int_\alpha \mathrm{e}^{-i\varepsilon_\alpha t}\cdot \frac{c_{\beta\alpha}(\pm)\, d_\pm(\alpha)}{\varepsilon_\beta - \varepsilon_\alpha \mp i0}\, |\beta\rangle \tag{12}$$

where the expansions (1) and (7) have been used. We now assume that all singularities in the expansion coefficients in (1) are taken care of by the energy denominator and that $c_{\beta\alpha}(\pm)$ and $d_+(\alpha)$ satisfy some conditions of smoothness and boundedness. The exact formulation of these conditions will be given in the appendix. There a justification will also be given of the formal steps in the following proof. Taking the scalar product of $|\varphi(t)\rangle$ with $|\psi_\pm(t)\rangle$ as given in (9) the first term on the right hand side of (12) gives one, because the states $|\alpha\rangle$ are a.o. The second term can be written in the form

$$\int_{\gamma\beta}\int_{\alpha} c_{\beta\alpha}(\pm)\, d_\pm(\alpha)\, \mathrm{e}^{i(\varepsilon_\gamma-\varepsilon_\beta)t} \langle\gamma\,|\,\beta\rangle \frac{\mathrm{e}^{i(\varepsilon_\beta-\varepsilon_\alpha)t}}{\varepsilon_\beta-\varepsilon_\alpha\mp i0}\cdot d_\pm^*(\gamma) \qquad (13)$$

The product $\langle\gamma|\beta\rangle$ may be replaced by $\delta(\gamma-\beta)$ in the limit $t\to\mp\infty$. Since the formal identities

$$\lim \frac{\mathrm{e}^{i(\varepsilon_\beta-\varepsilon_\alpha)t}}{\varepsilon_\beta-\varepsilon_\alpha-i0} = \begin{matrix} 2\pi i\,\delta(\varepsilon_\beta-\varepsilon_\alpha) & \text{for } t\to+\infty \\ 0 & \text{for } t\to-\infty \end{matrix} \qquad (14)$$

and

$$\lim \frac{\mathrm{e}^{i(\varepsilon_\beta-\varepsilon_\alpha)t}}{\varepsilon_\beta-\varepsilon_\alpha+i0} = \begin{matrix} 0 & \text{for } t\to+\infty \\ -2\pi i\delta(\varepsilon_\beta-\varepsilon_\alpha) & \text{for } t\to-\infty \end{matrix} \qquad (15)$$

will also be proved in the appendix, it follows that the expression in (13) tends to zero for $t\to\mp\infty$. This proves (11).

We have therefore shown that for asymptotic times the state $|\varphi(t)\rangle$ can be represented in the form $|\psi_\pm(t)\rangle$ (equation (9)). This means that the states $|\alpha\rangle$ are indeed a.s. From (9) we see that a possible choice for $b(\alpha)$ and $\tilde{b}(\alpha)$ in (4) and (5) is $d_+(\alpha)$ and $d_-(\alpha)$ respectively. We will show that this choice is unique. Suppose there is another $b'(\alpha)$ such that in addition to (4) also

$$|\varphi(t)\rangle = \int_\alpha b'(\alpha)\,\mathrm{e}^{-i\varepsilon_\alpha t}\,|\alpha\rangle \quad \text{for} \quad t\to-\infty$$

tends to zero in norm. Then for any state

$$|\chi(t)\rangle = \int_\alpha c(\alpha)\,\mathrm{e}^{-i\varepsilon_\alpha t}\,|\alpha\rangle$$

we have, because the states $|\alpha\rangle$ are a.o.,

$$\lim_{t\to-\infty} \langle\chi(t)|\varphi(t)\rangle = \int_\alpha c^*(\alpha)\,b(\alpha) = \int_\alpha c^*(\alpha)\,b'(\alpha).$$

The last two terms in this expression define a scalar product in a new Hilbert space of L^2 functions, which is the direct sum of as many Hilbert spaces as there are channels. Since in the above equality the $c(\alpha)$ that are admitted (see appendix) form a dense set in this new Hilbert space, it follows that $b(\alpha) = b'(\alpha)$ (almost everywhere). In the same way one can prove that $\tilde{b}(\alpha)$ is unique. The S-matrix is therefore defined by

$$d_-(\alpha) = \int_\beta S_{\alpha\beta} d_+(\beta) \qquad (16)$$

4. *Unitarity and form of the S-matrix.* In the same way as we proved (11), it can be shown, using all equalities in (14) and (15), that the following relations hold:

$$\lim_{t\to+\infty} \langle\psi_+(t)|\varphi(t)\rangle = \int_\alpha d^*_+(\alpha)\, d_-(\alpha) = \tag{A}$$
$$= \int_{\beta\alpha} d^*_+(\beta)[\delta(\beta-\alpha) - 2\pi i c_{\beta\alpha}(+)\,\delta(\varepsilon_\beta - \varepsilon_\alpha)]\, \mathrm{d}_+(\alpha)$$

$$\lim_{t\to-\infty} \langle\psi_+(t)|\varphi(t)\rangle = 1 \tag{B}$$
$$= \int_{\alpha\beta} d^*_+(\beta)[\delta(\beta-\alpha) + 2\pi i c_{\beta\alpha}(-)\cdot\delta(\varepsilon_\beta - \varepsilon_\alpha)]\, d_-(\alpha)$$

$$\lim_{t\to+\infty} \langle\psi_-(t)|\varphi(t)\rangle = 1$$
$$= \int_{\beta\alpha} d^*_-(\beta)[\delta(\beta-\alpha) - 2\pi i c_{\beta\alpha}(+)\,\delta(\varepsilon_\beta - \varepsilon_\alpha)]\, d_+(\alpha) \tag{C}$$

$$\lim_{t\to-\infty} \langle\psi_-(t)|\varphi(t)\rangle = \int_\alpha d^*_-(\alpha)\, d_+(\alpha)$$
$$= \int_{\beta\alpha} d^*_-(\beta)[\delta(\beta-\alpha) + 2\pi i c_{\beta\alpha}(-)\,\delta(\varepsilon_\beta - \varepsilon_\alpha)]\, d_-(\alpha) \tag{D}$$

For the following it will be useful to define operators L^+ and L^- in the Hilbertspace of functions $d(\alpha)$ by their matrixelements

$$L^\pm_{\beta\alpha} = \delta(\beta-\alpha) \mp 2\pi i c_{\beta\alpha}(\pm)\,\delta(\varepsilon_\beta - \varepsilon_\alpha) \tag{17}$$

Moreover, it will be advantageous to use abbreviations for the expressions in (A), (B), (C) and (D) by introducing the bracket notation

$$(c, L^\pm d) = \int_{\alpha\beta} c^*(\alpha)\, L^\pm_{\alpha\beta}\, d(\beta).$$

Faddeev[3]) has shown (theorem 9.2) that the operator S defined in (16) is isometric and maps the entire Hilbertspace of L^2 functions of our type $d(\alpha)$ (his formula 9.6) onto itself (theorem 9.1). This is equivalent to his S-matrix being unitary. We now want to prove that

$$S = L^+ \tag{18}$$

$$S^{-1} = S^\dagger = L^- \tag{19}$$

We first of all remark that S is defined everywhere, but that the operators $L^\pm$ are defined only on the dense subset of smooth and finite functions $d(\alpha)$. From (A) and (16) follows that for these functions

$$(d_+, d_-) = (d_+, Sd_+) = (d_+, L^+d_+). \tag{20}$$

Substituting for d_+ the forms $c_1 + c_2$ and $c_1 + ic_2$, where c_1 en c_2 are again smooth and finite, we obtain

$$(c_1, (S - L^+)\, c_2) = 0 \tag{21}$$

(21) shows that $S - L^+$ is bounded on its domain. It can therefore be uniquely to an everywhere defined bounded operator. Since S is defined already on the extension of this domain it follows immediately that $S = L^+$, or in matrixform

$$S_{\alpha\beta} = \delta(\alpha - \beta) - 2\pi i c_{\alpha\beta}(+)\,\delta(\varepsilon_\alpha - \varepsilon_\beta). \tag{22}$$

In the same way one proves from (D) that $S^{-1} = L^-$, or

$$S^{-1}_{\alpha\beta} = \delta(\alpha - \beta) + 2\pi i\, c_{\alpha\beta}(-)\,\delta(\varepsilon_\alpha - \varepsilon_\beta). \tag{23}$$

From the last two equations and the unitarity of S it follows that on the energy shell

$$c_{\alpha\beta}(+) = c^*_{\beta\alpha}(-). \tag{24}$$

5. *Three-particle systems.* In this section we will prove explicitly that the states $|\alpha\rangle$ for three-particle systems, as defined in section 2, are indeed a.o. and a.s. Consider the wavefunctions

$$\varphi_1(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, t) = (2\pi)^{-\frac{9}{2}} \int c(\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3)\cdot \mathrm{e}^{i(\boldsymbol{k}_1\cdot\boldsymbol{r}_1+\boldsymbol{k}_2\cdot\boldsymbol{r}_2+\boldsymbol{k}_3\cdot\boldsymbol{r}_3-\varepsilon_\alpha t)}\,\mathrm{d}\boldsymbol{k}_1\,\mathrm{d}\boldsymbol{k}_2\,\mathrm{d}\boldsymbol{k}_3 \tag{25}$$

and

$$\varphi_2(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, t) = \psi_n(\boldsymbol{r}_{23}) \int \mathrm{d}(\boldsymbol{k}_1\boldsymbol{K}_{23})(2\pi)^{-3}\cdot \mathrm{e}^{i(\boldsymbol{k}_1\boldsymbol{r}_1+\boldsymbol{K}_{23}\boldsymbol{R}_{23}-\varepsilon_\beta t)}\,\mathrm{d}\boldsymbol{k}_1\,\mathrm{d}\boldsymbol{K}_{23} \tag{26}$$

which belong to two different channels and where $\boldsymbol{r}_{23} = \boldsymbol{r}_2 - \boldsymbol{r}_3$,

$$\boldsymbol{R}_{23} = \frac{m_2\boldsymbol{r}_2 + m_3\boldsymbol{r}_3}{m_2 + m_3}$$

and n specifies the bound state of particle 2 and 3 with energy E_n ·

$$\varepsilon_\alpha = \frac{\hbar^2k_1^2}{2m_1} + \frac{\hbar^2k_2^2}{2m_2} + \frac{\hbar^2k_3^2}{2m_3} \quad \text{and}$$

$$\varepsilon_\beta = \frac{\hbar^2k_1^2}{2m_1} + \frac{\hbar^2\boldsymbol{K}_{23}^2}{2(m_2 + m_3)} - |E_n|.$$

We want to show that:

$$\lim_{t\to\pm\infty} \int \varphi_1^*(\boldsymbol{r}_1\boldsymbol{r}_2\boldsymbol{r}_3\, t)\,\varphi_2(\boldsymbol{r}_1\boldsymbol{r}_2\boldsymbol{r}_3 t)\,\mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2\,\mathrm{d}\boldsymbol{r}_3 = 0 \tag{27}$$

In order to do this, we first expand $\psi_n(\boldsymbol{r}_{23})$ into plane waves $(2\pi)^{-\frac{3}{2}}\cdot \mathrm{e}^{i\boldsymbol{k}_{23}\cdot\boldsymbol{r}_{23}}$. By transforming from the variables $(\boldsymbol{K}_{23}, \boldsymbol{k}_{23})$ to $(\boldsymbol{k}_2, \boldsymbol{k}_3)$ such that

$$\boldsymbol{K}_{23} = \boldsymbol{k}_2 + \boldsymbol{k}_3 \quad \text{and} \quad \boldsymbol{k}_{23} = \frac{m_3\boldsymbol{k}_2 - m_2\boldsymbol{k}_3}{m_2 + m_3},$$

we can apply the theorem of Fourier-Plancherel to the $(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)$ –integration and obtain for the integral in (27) the following

$$\int c^*(\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{k}_3)\, \hat{\psi}_n\, (\boldsymbol{k}_{23})\, \mathrm{d}(\boldsymbol{k}_1, \boldsymbol{K}_{23})\, \mathrm{e}^{i(\varepsilon_\alpha - \varepsilon_\beta)t}\, \mathrm{d}\boldsymbol{k}_1\, \mathrm{d}\boldsymbol{k}_2\, \mathrm{d}\boldsymbol{k}_3, \tag{28}$$

where

$$\varepsilon_\alpha - \varepsilon_\beta = + \frac{\hbar^2 k_{23}^2}{2m_{23}} + |E_n|.$$

The integrand is a L^1-function. After a transformation to new variables, of which $\varepsilon_\alpha - \varepsilon_\beta$ is one, the integrand is again a L^1-function, so that according to Fubini's theorem[6]), repeated integration is permitted. Performing all integrations except over $\varepsilon_\alpha - \varepsilon_\beta = u$ gives an integral of the form $\int f(u)\, \mathrm{e}^{iut}\, \mathrm{d}u$. Since $f(u)$ is (again by Fubini) a L^1-function, this integral approaches zero for $t \to \pm\infty$, due to the Riemann-Lebesgue theorem. This proves (27) for a special case. When φ_1 and φ_2 belong to two different bound state channels the proof can be given along the same lines as in the previous example. We conclude therefore that the states $|\alpha\rangle$ in the three-particle case are a.o. In section 2 it was shown that the states $|\alpha\rangle$ are a.s. when certain conditions on $c_{\beta\alpha}(\pm)$ and $d_\pm(\alpha)$ are satisfied. In the appendix, it will be proved that sufficient conditions are:

Ia. $c(\beta, \alpha)$ is Hölder continuous in all variables (α, β)

Ib. $|c(\beta, \alpha)| \leqslant M.\ \varepsilon_\beta^{-3}$ for $\varepsilon_\beta \to \infty$ if α is restricted to a finite domain.

II. $d_+(\alpha)$ is Hölder continuous in α with finite support.

This last condition is not an actual restriction, because the set of functions $d(\boldsymbol{k}_1, \boldsymbol{k}_{23})$ is dense, so that the proof of the unitarity of the S-matrix as given in section 4 still holds. The question therefore whether the states $|\alpha\rangle$ are asymptotically stationary all depends on the possibility to satisfy I. It has not been investigated whether the Schrödinger equation allows solutions $c(\beta, \alpha)$ which indeed fulfil this condition.

6. *Conclusions.* In this paper we have developed an S-matrix formalism to describe the scattering of compound many-particle systems. Since in a scattering experiment the initial and final states are always products of one-particle states – each of which may be either elementary or composite – we introduced these product states as the basic states of our Hilbert space. In this way the definition of the S-matrix becomes very simple, but the proof of the uniqueness and of the unitarity of this S-matrix is complicated by the fact that these product states are overcomplete. The proof, which uses a theorem of Faddeev[3]), could nevertheless be given by first showing that our basic states are asymptotically orthonormal and asymptotically stationary, concepts which were introduced by Van Hove[1]) for many-particle systems. The remaining problem was to show that in principle our S-matrix could be calculated from the stationary scattering states. For this purpose these stationary scattering states were expanded into our (over-

complete) basic set of product states. (See equation (1)). The expansion coefficients $c_{\beta\alpha}(+)$ are of course not uniquely defined, but it could be shown that on the energy shell (i.e. for $\varepsilon_\beta = \varepsilon_\alpha$) they are simply related to the S-matrix (equation (22)) so that there is no ambiguity for that case. The relation (22) is the same as obtained in ordinary two-particle scattering theory. The only condition we had to impose on the function $c_{\alpha\beta}(+)$, in order to prove that our product states were indeed asymptotically stationary, was that is satisfied a Hölder condition in all variables. It remains an open question, which has neither been solved in Faddeev's work, whether the Schrödinger equation for the stationary scattering state allows a solution so that the Hölder condition for $c_{\alpha\beta}(+)$ is fulfilled. For an investigation of this problem the (modified) Faddeev equations for $c_{\alpha\beta}(+)$ should first be derived. This will be done in the following paper[4]).

MATHEMATICAL APPENDIX

In this appendix we will prove the validity of the following formal identities:

A. $$\lim_{t_0\to\pm\infty} \frac{e^{i\omega t_0}}{\omega + i0} = \begin{cases} 0 & \text{for } t_0 \to +\infty \\ -2\pi i\delta(\omega) & \text{for } t_0 \to -\infty \end{cases} \qquad \text{A.1)}.$$

$$\lim_{t_0\to\pm\infty} \frac{e^{i\omega t_0}}{\omega - i0} = \begin{cases} +2\pi i\delta(\omega) & \text{for } t_0 \to +\infty \\ 0 & \text{for } t_0 \to -\infty \end{cases} \qquad \text{(A.2)}$$

B. Formulate under what conditions on the functions $c(\beta, \alpha)$ and $d_+(\alpha)$ the asymptotic stationarity can be proved.

A. Let $f(\omega)$ be a Hölder-continuous function with finite support:

$$|f(\omega + h) - f(\omega)| \leqslant C\,|h|^\nu \text{ with } 0 < \nu < 1 \text{ and } f(\omega) = 0 \text{ if } |\omega| \geqslant a.$$

We have

$$\int_{-\infty}^{\infty} \frac{e^{i\omega t_0}}{\omega + i\varepsilon} f(\omega)\, d\omega = -\sqrt{2\pi}\cdot i. \int_0^\infty e^{-\varepsilon t} \hat{f}(t - t_0)\, dt \qquad \text{(A.3)}$$

by the theorem of Parseval, where

$$\hat{f}(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(\omega)\, e^{-i\omega t}\, d\omega.$$

The function $\hat{f}(t)$ is in $C^{(\infty)}$ (infinitely often differentiable) and bounded. If in (A.3) the limit $\varepsilon \downarrow 0$ could be taken inside the integral sign, we would have proved (A.1). However, simple examples show that $\hat{f}(t)$ is in general not in L', so the Lebesgue theorem on bounded convergence cannot be used here. Therefore we proceed as follows: $f(\omega)$ can be approximated uniformly by triangle functions

$$\begin{aligned}\Delta(\omega) &= 0 \quad \omega < a. \\ &= -a + \omega \quad a \leqslant \omega \leqslant b \\ &= -\omega - a + 2b \quad b \leqslant \omega \leqslant 2b - a. \\ &= 0 \quad \omega \geqslant 2b - a.\end{aligned}$$

thus: $|f(\omega) - f_n(\omega)| < \eta$ if $n \geqslant N_0$.

Since $I = \lim_{n\to\infty} \lim_{t_0\to\pm\infty} \lim_{\varepsilon\downarrow 0} \int_{-\infty}^{\infty} \frac{f_n(\omega)}{\omega + i\varepsilon} e^{i\omega t_0} d\omega = \lim_{t_0\to\pm\infty} \lim_{\varepsilon\downarrow 0} \int_{-\infty}^{\infty} \frac{f(\omega) e^{i\omega t_0} d\omega}{\omega + i\varepsilon}$

and since the Fourier transform of a finite sum of triangle functions, is a Riemann-integrable function, we have by (A.3):

$$I = \lim_{n\to\infty} \lim_{t_0\to\pm\infty} - \sqrt{2\pi}\cdot i\cdot \int_0^{\infty} \hat{f}_n(t - t_0)\, dt =$$

$$= \lim_{n\to\infty} -\sqrt{2\pi}\cdot i\cdot \int_{-\infty}^{\infty} \hat{f}_n(t)\, dt = \begin{cases} -2\pi i\cdot f(0) & \text{if } t_0 \to -\infty. \\ 0 & \text{if } t_0 \to +\infty.\end{cases}$$

And this proves (A.1). In the same way one proves (A.2).

B. We now consider integrals of the form (see e.g. (13)):

$$I(t) = \int_{\beta\gamma} e^{i\varepsilon_\gamma t} g^*(\gamma) \left[\int_\alpha \frac{c_{\beta\alpha}(+)\, d(\alpha)\, e^{-i\varepsilon_\alpha t}}{\varepsilon_\beta - \varepsilon_\alpha - i0} \right] \langle\gamma|\beta\rangle \tag{B.1}$$

where α, β and γ belong to three arbitrary channels C_α, C_β and C_γ.

In order for the integral between square brackets, which we denote by $F(\beta)$, to exist, we impose the following conditions on $c_{\beta\alpha}(+)$ and $d(\alpha)$, $g(\gamma)$. (for explicit formula's for 3-particle systems, see section 5):

Conditions: $c_{\beta\alpha}(+)$ is Hölder continuous (H.C.) in (β, α)
$d(\alpha)$ and $g(\gamma)$ are H.C. with finite support.

Then $F(\beta)$ exists for all β, since integration over the angles of α leaves a H.C. function in $(\beta, \varepsilon_\alpha)$. This statement is true because $d(\alpha)$ has finite support. The remaining integration over ε_α can then be performed. $F(\beta)$ is even H.C. in β (for a proof we can use the theorem of Privalov-Plemelj[5])).

If $F(\beta)$ is in L^2, $\int_\beta F(\beta) \langle\gamma|\beta\rangle$ gives a L^2-function of γ. In $I(t)$ of $(B.1)$, the subsequent integration over γ is then defined since we have the scalar product of two L^2-functions.

In order that $F(\beta)$ is in L^2 it is sufficient that in the case of 3 particles $|c_{\beta\alpha}^{(+)}| \leqslant M\varepsilon_\beta^{-3}$ for $\varepsilon_\beta \to \infty$, if α is restricted to a finite domain. In theorem

(9.2) sub 1 Faddeev[3]) proves more generally that for 3 particles $F(\beta)$ is in L^2. We have therefore proved that under very general conditions for $c_{\beta\alpha}(+)$ the function $I(t)$ exists for all t. We must now consider the limit $t \to \pm\infty$.

B I. If the channels C_β and C_γ are equal, $\langle\gamma|\beta\rangle = \delta(\gamma - \beta)$, the bound states if present drop away by integration, and (B.1) reduces to:

$$I(t) = \int\limits_\beta e^{i\varepsilon_\beta t} g^*(\beta) \left[\int\limits_\alpha \frac{c_{\beta\alpha}(+)\cdot d(\alpha)\, e^{-i\varepsilon_\alpha t}}{\varepsilon_\beta - \varepsilon_\alpha - i0} \right] \tag{B.2}$$

We will now prove that $I(t) = J(t)$ with

$$J(t) = \int\limits_{\varepsilon_\beta - \varepsilon_\alpha} \frac{e^{i(\varepsilon_\beta - \varepsilon_\alpha)t}}{\varepsilon_\beta - \varepsilon_\alpha - i0} \left\{ \int\limits_{\alpha\beta} g^*(\beta)\, c_{\beta\alpha}(+)\, d(\alpha) \right\} \tag{B.3}$$

where the prime indicates that we integrate only over the angles in α, β and over ε_α, but with fixed $\varepsilon_\beta - \varepsilon_\alpha$. The expression in (B.3) exists, since the numerator in (B.5) is Hölder continuous in $(\varepsilon_\beta - \varepsilon_\alpha)$. We must therefore show that in the limit $\varepsilon \downarrow 0$ the integral:

$$\int\limits_\beta e^{i\varepsilon_\beta t}\, g^*(\beta) \left[\int\limits_\alpha c(\beta, \alpha)\, d(\alpha)\, e^{-i\varepsilon_\alpha t} \left(\frac{1}{\varepsilon_\beta - \varepsilon_\alpha - i\varepsilon} - \frac{1}{\varepsilon_\beta - \varepsilon_\alpha - i0} \right) \right.$$

tends to zero. For this purpose it is sufficient to prove that

$$K(\beta, \varepsilon_\beta) = \int\limits_\beta c(\beta, \alpha)\, d(\alpha)\, e^{-i\varepsilon_\alpha t} \left(\frac{1}{\varepsilon_\beta - \varepsilon_\alpha - i\varepsilon} - \frac{1}{\varepsilon_\beta - \varepsilon_\alpha - i0} \right)$$

approaches zero uniformly in β. Integration over the angles of α gives (all for fixed t).

$$K(\beta, \varepsilon_\beta) = \int G(\text{angles of } \beta, \varepsilon_\beta, \varepsilon_\alpha,) \left(\frac{1}{\varepsilon_\beta - \varepsilon_\alpha - i\varepsilon} - \frac{1}{\varepsilon_\beta - \varepsilon_\alpha - i0} \right) d\varepsilon_\alpha,$$

where G is H.C. in all its variables.

It can then indeed be shown that $|K(\beta, \varepsilon)|$ can be made smaller then any given number and uniformly in β by taking ε small enough. This proves $I(t) = J(t)$ for all t.

In order to apply (A.2) to (B.3) we must first show that

$$H(\varepsilon_\beta - \varepsilon_\alpha) = \int\limits_{\alpha\beta} g^*(\beta)\, c(\beta, \alpha)\, d(\alpha) \tag{B.4}$$

is H.C. in $\varepsilon_\beta - \varepsilon_\alpha$ and has finite support. The latter follows from the fact that both $g(\beta)$ and $d(\alpha)$ have finite support.

To prove the H.C. for $H(\varepsilon_\beta - \varepsilon_\alpha)$ we note that repeated integration in

(B.4) is permitted. The integration over the angles of α gives a H.C. function in ε_α because the surface in α-space of $\varepsilon_\alpha =$ constant is bounded. This follows from the fact that d(α) has finite support. In the same way we see that the integration over the angles of β gives a H.C. function in ε_β. By changing the last variables $(\varepsilon_\alpha, \varepsilon_\beta)$ to $(\varepsilon_\alpha, \varepsilon_\beta - \varepsilon_\alpha)$ we still have a H.C. function in ε_α and $\varepsilon_\beta - \varepsilon_\alpha$.

Integration over ε_α for fixed $\varepsilon_\beta - \varepsilon_\alpha$ leaves us with $H(\varepsilon_\beta - \varepsilon_\alpha)$ which is then H.C. Application of (A.2) to (B.3) now gives

$$\lim I(t) = \begin{cases} 2\pi i \int\limits_{\alpha\beta} g^*(\beta)\, c(\beta, \alpha)\, \mathrm{d}(\alpha)\, \delta(\varepsilon_\beta - \varepsilon_\alpha) & \text{for} \quad t \to +\infty \\ 0 & \text{for} \quad t \to -\infty \end{cases} \tag{B.5}$$

B II. If C_β is different from C_γ, the integral in (B.1) will give zero for $t \to \pm\infty$. We will prove this with the Liemann-Lebesgue theorem. As in B I the limit $\varepsilon \downarrow 0$ which is implied in (B I) can be taken before all integrattions. Repeated integration is again permitted. The reason here is different from the reason in the case B I. There the integrand was finite and continuous. Here, however, the integrand contains the Fourier transforms of the bound state wave functions and these are not necessarily continuous. Repeated integration in nevertheless permitted by a theorem on Lebesque integration[6]) if the integrand is in L'. This condition is indeed satisfied since our integrand is a product of two L^2 functions.

Received 27-6-66

REFERENCES

1) Van Hove, L., Physica **21** (1955) 901 and **22** (1956) 343.
2) Faddeev, L. D., JETP **12** (1960) 1204.
Soviet Physics – Doklady **6** (1961) 384; **7** (1962) 600.
3) Faddeev, L. D., Mathematical aspects of the three-body problem in the quantum scattering theory (Israël Program for Scientific Translations, Jerusalem, 1965).
4) Malfliet, R. and Ruijgrok, Th., Physica **33** (1967) 607.
5) Mushkhelishvili, Singular integral equations, section 19 (Noordhoff).
6) Burkill, J. C. The Lebesque Intergral, (Cambridge University Press, 1951) page 64.