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ON THE RELATION BETWEEN THE TIME-DEPENDENT AND STATIONARY TREATMENTS OF COLLISION PROCESSES

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Introduction.

In recent years, the notion of the S-matrix has found an increasing application in the treatment of collision processes, both in nuclear problems and field theory. In the numerous papers on this subject, the definition of the S-matrix itself has, however, not always been the same, and the connection between the different definitions has not always been quite clear.

When the treatment of the collision process is based on the Schrödinger equation, different definitions of the S-matrix suggest themselves, according as the treatment is based on the time-independent or the time-dependent Schrödinger equation. In the first case, one is led to the original Heisenberg definition; in the latter case, to DYSON's definition of the S-matrix. On the other hand, if one starts from the equations of motion (the field equations) in a Heisenberg representation instead of using the Schrödinger equation, another method of defining the S-matrix suggests itself, which was developed by KÄLLÉN and by YANG and FELDMAN and which has proved very convenient in various field theories.

In the present paper, an attempt has been made to correlate the various methods and to discuss which results can be derived without use of expansions in powers of the interaction, which results are valid as long as such expansions converge, and which results can be valid only as long as the possibility of bound states may be ignored.

I. Notation.

In order to facilitate derivations, and to condense formulas of n'th order perturbation theory to a printable, inspectional, and manageable size, we introduce a symbolic notation, as follows.

Let A, B, C, ... be q-numbers, represented by matrices with a left-hand label L and a right-hand label R, indicating rows and columns, respectively. In DIRAC's bracket notation,

$$A = BC \text{ means } \langle L|A|R\rangle = \int \langle L|B|k\rangle\, dk\, \langle k|C|R\rangle. \quad (1.1)$$

In most cases, we shall use for k a set of q-numbers commuting with each other and with the unperturbed ("free particle") energy E of the particles considered. For instance, k may be the momenta of the particles, or a set of occupation numbers.

In the following,

$$A = B f(E_L, E_R) \text{ means } \langle L|A|R\rangle = \langle L|B|R\rangle \cdot f(E_L, E_R) \quad (1.2)$$

in any representation in which E may be considered a function of the variables used for labels L and R. Between braces, however, L and R refer to the positions farthest to the left and to the right between such braces; thus,

$$A\{B \cdot f(E_L, E_R)\} = C \text{ means}$$

$$\int \langle L|A|k\rangle\, dk\, \langle k|B|R\rangle\, f(E_k, E_R) = \langle L|C|R\rangle. \quad (1.3)$$

We shall put

$$E_{ij} \equiv E_i - E_j = -E_{ji}. \quad (1.4)$$

Often we shall write a product of q-numbers and insert between or beside the factors one symbol $\|$ (pronounced "gage") and several symbols δ ("delt"), $'$ ("dash"), § ("scat"), $\flat$ ("flat"), and ? (pronounced "slash"). If G denotes the position of the gage between or beside the q-numbers, these symbols are to be interpreted as follows:

$$\left.\begin{aligned} &\text{Each delt at position } \Delta \text{ stands for a} \\ &\qquad \text{factor } -i\pi\delta(E_G - E_s) = (\pi/i)\,\delta(E_{G\Delta}). \\ &\text{Each dash at position } d \text{ stands for a} \\ &\qquad \text{factor } D_{Gd} \equiv E_{Gd}/(E_{Gd}^2 + a^2) = -D_{dG}. \end{aligned}\right\} \quad (1.5)$$

$$\left.\begin{aligned}&\text{Each scat at position } S \text{ stands for a}\\&\qquad\text{factor } \S\,(E_{GS}) \equiv (E_G - E_S + i\alpha)^{-1}.\\&\text{Each flat at position } F \text{ stands for a}\\&\qquad\text{factor } \flat\,(E_{GF}) \equiv (E_G - E_F - i\alpha)^{-1}.\end{aligned}\right\} \tag{1.5}$$

In (1.5), α is an infinitely small, real, positive number. At the end of each calculation we take $\alpha \to 0$. (Occasionally, α has a physical meaning and the convenient mathematical limit $\alpha \to 0$ is only a good *approximation*, as the physical α is small, but not really zero).

The dash, flat, and scat at position K are easily recognized as three ways of dividing by $E_{GK} \equiv E_G - E_K$; if the quantity divided does not vanish for $E_G = E_F$, the results of these three different divisions differ by delta functions, as discussed below (see Eq. (1.9)). If we do not want to specify which of these three methods of division we have in mind, we indicate division by $(E_G - E_K)$ by a gage ($\|$) at position G and a slash (?) at position K.

If $\dagger$ denotes the Hermitian conjugate of a matrix.

$$\langle L \,|\, A^\dagger \,|\, R\rangle = \langle R \,|\, A \,|\, L\rangle^*, \tag{1.6}$$

then the following rules are obvious:

1. *Rules valid if A and B are any expressions containing any dashes, scats, flats, slashes or delts:*

$$\left.\begin{aligned}{}'A\| &= {}^1\!/_2\,(\S\, A\| + \flat\, A\|),\\ (A\|)\,(\delta B\|) &= A\delta B\|,\\ \delta A\| &= \|\, A\delta,\\ ('A\|)^\dagger &= \|\,(A^\dagger)',\\ (\delta A\|)^\dagger &= -\|\,(A^\dagger)\delta = -\delta A^\dagger\|,\\ (\S\, A\|)^\dagger &= \|\,(A^\dagger)\,\flat,\\ (\flat\, A\|)^\dagger &= \|\,(A^\dagger)\,\S.\end{aligned}\right\} \tag{1.7}$$

In general, the rule, that the Hermitian conjugate of a product equals the product in reversed order of sequence of the Hermitian conjugates of the factors, applies also to products interjected with a gage and various delts, dashes, etc., as long as we treat these symbols as factors themselves and as long as we put

$$(')^\dagger = ', \qquad (\delta)^\dagger = -\delta, \qquad (\S)^\dagger = \flat, \qquad (\flat)^\dagger = \S. \tag{1.8}$$

A further general rule is

$$\S A\| = 'A\| + \delta A\|; \qquad \flat A\| = 'A\| - \delta A\|. \tag{1.9}$$

This rule is easily verified by multiplying these equations by an arbitrary function of E_{RL} continuous along the real axis, and integrating them in the complex E_{RL} plane along the real axis, taking the limit $a \to 0$ at the end. If $C(a)$ is a path of integration from the minimum value of E_{RL} to a point $(E_{RL})_{\min} - ia$, then parallel to the real axis to the point $-(i+1)a$, then along a semi-circle through 0 to $+(1-i)a$, and from there again at a constant distant a below the real axis to $+\infty$, then

$$\left.\begin{aligned} \int_{(E_{RL})\,\min}^{\infty} (\S A\|)\, f(E_{RL})\, dE_{RL} &= \lim_{a\to 0} \int_{C(a)} A \frac{f(E_{RL})}{E_{RL} + ia}\, dE_{RL} \\ &= P\int A \frac{f(E_{RL})}{E_{RL}}\, dE_{RL} - i\pi f(0)\, A\,\big|_{E_R = E_L}, \end{aligned}\right\} \tag{1.10}$$

where P is the Cauchy principal value of the integral along the real axis, and where the last term derives from the integral in clockwise (negative) direction around the pole at $-ia$. Similarly, we prove

$$\left.\begin{aligned} \int_{(E_{RL})\,\min}^{\infty} (\flat A\|)\, f(E_{RL})\, dE_{RL} &= P\int A \frac{f(E_{RL})}{E_{RL}}\, dE_{RL} \\ &\quad + \pi i f(0)\, A\,\big|_{E_R = E_L}. \end{aligned}\right\} \tag{1.11}$$

So, by the first equation (1.7),

$$\int ('A \,\|\,) f(E_{RL})\, dE_{RL} = P\int A \frac{f(E_{RL})}{E_{RL}} dE_{RL}, \qquad (1.12)$$

and by (1.5),

$$\int (\delta A \,\|\,) f(E_{RL})\, dE_{RL} = -i\pi f(0)\, A\,|_{E_R = E_L}. \qquad (1.13)$$

From the validity of Eqs. (1.10) — (1.13) for *arbitrary* $f(E_{RL})$ we conclude to the relations (1.9). Also, subtracting $\S(E_{RL})$ and $\flat(E_{RL})$, we get from (1.5)

$$\left.\begin{aligned} \S(E_{RL}) - \flat(E_{RL}) &= \frac{1}{E_{RL} + ia} - \frac{1}{E_{RL} - ia} \\ &= \frac{-2ia}{E_{RL}^2 + a^2} \to -2\pi i \delta(E_{RL}) \end{aligned}\right\} \quad (1.9\,a)$$

for $a \to 0$, in accordance with (1.9).

2. *Rules valid only if q is a q-number not containing any other delts, dashes, scats, flats or slashes referring to the same gage*:

$$\left.\begin{aligned} {}'q\,\| &= -\|\, q', \\ \S q\,\| &= -\|\, q\flat, \\ \flat q\,\| &= -\|\, q\S, \\ ?q\,\| &= -\|\, q(?^\dagger), \\ (?q\,\|\,)^\dagger &= -?(q^\dagger)\,\|. \end{aligned}\right\} \quad (1.14)$$

The latter three equations easily follow from the first one together with (1.8) and (1.7).

We might have started from Eqs. (1.10) — (1.13) as *definitions* of the scat, flat, dash, and delt. This kind of definition, however, easily creates confusion, as shown by the following example which is of importance also for its applications.

Consider the algebraic identity

$$\left.\begin{aligned}&(E_{LR}\,E_{LM})^{-1}+(E_{RM}\,E_{LM})^{-1}+(E_{RM}\,E_{RL})^{-1}\\&=(E_{LR}\,E_{LM}\,E_{RM})^{-1}(E_{RM}+E_{LR}-E_{LM})=0.\end{aligned}\right\}\quad(1.15)$$

If the dash is defined by (1.12), Eq. (1.15) easily creates the wrong impression that

$$F\equiv\|A'\,B'+{}'A\,\|\,B'+{}'A\,{}'B\,\|\qquad(1.16)$$

would vanish. (In fact, of course, such conclusion cannot be drawn even from (1.12), as the "principal value" to be taken in the double integrations over the energies of the intermediate state M (due to Eq. (1.1)) and of the final L in $P\int dE_L\,f(E_L)\,F$ would be defined differently for each of the three terms in (1.16).) In the Appendix A it is shown that, instead of the vanishing of F, we have the important relation

$$D_{LR}\,D_{LM}+D_{RM}\,D_{LM}+D_{RM}\,D_{RL}=\pi^2\,\delta(E_{LM})\,\delta(E_{MR}),\qquad(1.17)$$

which means

$$\left.\begin{aligned}&\|A'\,B'+(\|A')\,({}'B\|)+{}'A\,{}'B\|\\&=\|A'\,B'+{}'A\|\,B'+{}'A\,{}'B\|=-\delta A\|\,B_\delta\end{aligned}\right\}\quad(1.18)$$

on account of (1.5).

If A is any matrix, we shall frequently in the following use the notation $A(t)$ for the time-dependent matrix

$$A(t)=A\exp(E_{RL}\,t/i\hbar).\qquad(1.19)$$

If A is the time-independent matrix representing an observable in Schrödinger representation, the $A(t)$ is the matrix representing this same observable in interaction representation. Obviously,

$$A(t)\;B(t)=(A\,B)\exp(E_{RL}\,t/i\hbar),\qquad(1.20)$$

since $E_{RM}+E_{ML}=E_{RL}$ if M is the position between the factors A and B. Thence, any algebraic relation between time-independent matrices remains valid if in both members of the equation all

matrices are replaced by the corresponding time-dependent matrices (1.19). Also by (1.6)

$$A(t)^{\dagger} = A^{\dagger} \exp(E_{RL}\, t/i\hbar) \equiv A^{\dagger}(t). \tag{1.21}$$

Obviously, all matrices of the form $\delta A \,\|$ are time-independent in interaction representation; that is

$$\delta A(t) \,\| = \delta A \,\| = \text{constant in time.} \tag{1.22}$$

It is sometimes useful to calculate the value of a time-dependent matrix $A(t)$ at $t \to \pm\infty$. If A has no singularities for $E_{RL} \to 0$, we may reason that $A(\pm\infty)$ vanishes, unless we prefer to maintain that $A(\pm\infty)$ has no well-defined value as $A(t)$ remains oscillatory. If the matrix considered is of the form $\S\, A(t) \,\|$, the result depends on the order of sequence of the limits $a \to 0$ and $t \to \pm\infty$. In this section, we consider the case that the limit $a \to 0$ is taken first. Then:

$$\left.\begin{aligned} &\lim_{\to \pm\infty} \int dE_{RL}\, f(E_{RL})\, \S\, A(t) \,\| \\ &= \lim_{t \to \pm\infty} \lim_{a \to 0} \int dE_{RL}\, \frac{f(E_{RL})}{E_{RL} + ia}\, A \exp(E_{RL}\, t/i\hbar) \\ &= \lim_{t \to \pm\infty} \lim_{a \to 0} \int_{-\infty}^{\infty} \frac{dx}{x + i\,|\,t\,|\,/\hbar}\, f(a\hbar x/|\,t\,|)\, A \exp(\pm ax/i). \end{aligned}\right\} \tag{1.23}$$

Before we take the limits any further, we perform the integration by closing the contour through $x = \mp i\,\infty$, where $\exp(\pm ax/i)$ vanishes. The pole at $x = -i\,|\,t\,|\,/\hbar$ is enclosed by the contour in the case of the upper signs only, so that

$$\lim_{t \to -\infty} \int dE_{RL}\, f(E_{RL})\, \S\, A(t) \,\| = 0, \tag{1.24}$$

$$\left.\begin{aligned} &\lim_{t\to+\infty}\int dE_{RL}\, f(E_{RL})\,\S A\,(t)\,\| \\ &= \lim_{t\to+\infty}\ \lim_{a\to 0}\left\{-2\pi i f(-ia)\,A\,\exp\,(-at/\hbar)\right\} \\ &= -2\pi i\, f(0)\,A\,|_{E_{RL}=0} = -2\pi i\int dE_{RL}\,\delta(E_{RL})f(E_{RL})\,A. \end{aligned}\right\} \quad (1.25)$$

As this is true for arbitrary functions $f(E_{RL})$, we conclude that

$$\S\, A\,(t\to-\infty)\,\| = 0; \qquad (1.26)$$

$$\S\ A\,(t\to+\infty)\,\| = 2\,\delta A\,\|\,, \qquad (at \ll 1). \qquad (1.27)$$

Similarly we show

$$\flat\, A\,(t\to-\infty)\,\| = -2\,\delta A\,\|, \qquad (a\,|\,t\,| \ll 1); \qquad (1.28)$$

$$\flat\, A\,(t\to+\infty)\,\| = 0. \qquad (1.29)$$

By (1.9) or

$$\left.\begin{aligned} \delta A\,\| &= {}^1\!/_2\,(\S\, A\,\| - \flat\, A\,\|), \\ {}'A\,\| &= {}^1\!/_2\,(\S\, A\,\| + \flat\, A\,\|), \end{aligned}\right\} \quad (1.30)$$

Eqs. (1.26)—(1.29) give the result

$$\delta A\,(t\to\pm\infty)\,\| = \delta A\,\|, \qquad (1.31)$$

which is trivial on account of (1.22), and

$${}'A\,(t\to\pm\infty)\,\| = \pm\,\delta A\,\|\,, \qquad a\,|\,t\,| \ll 1. \qquad (1.32)$$

Because of the ambiguity of the mathematical method used for arriving at the results (1.24)—(1.32), one should justify this method on physical grounds whenever these results are formally used. The main point in the above derivation is that the limit $t\to\pm\infty$ is taken last of all, while a in (1.25) had already been put equal to zero; otherwise, we would have found zero instead

of $\delta A \parallel$ in all right-hand members of (1.25)—(1.32). In other words, we have kept $a \mid t \mid$ small in the limits $t \to \pm \infty$ for arriving at the results (1.25)—(1.32). A justification or refutation of such procedure is possible only after we give a a physical meaning. Chapter IX deals with a different order of sequence of these limits.

II. Stationary states, scattering matrices, and Heisenberg's *S*-matrix.

In this chapter, we shall use the definition of HEISENBERG's *S*-matrix given earlier by one of us[4], but the quantities there denoted by W, U, and $\delta_+ (-x)$ are represented here by the notation E, $-2\pi i F$, and

$$\delta_+ (x) = \int_0^\infty \exp(ikx)\, dk/2\pi = {}^1/_2\, \delta(x) - P\left(\frac{1}{2\pi i x}\right). \qquad (2.1)$$

Here, P indicates that one should take the principal value in subsequent integrations over x. With this notation, and $\delta_- (x) = \delta(x) - \delta_+ (x)$, the meaning of the scat and of the flat by (1.10)—(1.11) can be represented by

$$\S\, A \parallel = -2\pi i\, \delta_+ (E_{RL})\, A; \qquad \flat\, A \parallel = 2\pi i\, \delta_- (E_{RL})\, A. \quad (2.2)$$

H will denote the total Hamiltonian of our system. It is the sum of the free particle energy E and the interaction V. In Schrödinger representation, these quantities are represented by matrices which for a closed system are time-independent, but the state vector (situation function, wave function) $\psi_S (t)$ is time-dependent and satisfies

$$i\hbar\, \partial \psi_S (t)/\partial t = H \psi_S (t) = (E + V)\, \psi_S (t). \qquad (2.3)$$

Let k again be a set of variables commuting with each other and with E. (For instance momenta, or occupation numbers). Starting from an arbitrary Schrödinger representation in q-space, we transform to interaction representation in k-space with wave function $\langle k \mid \psi (t)$ by the method of variation of constants (used also in time-dependent perturbation theory):

$$\psi_S(q, t) = \int \langle q \mid k \rangle \exp(Et/i\hbar)\, dk \langle k \mid \psi(t), \qquad (2.4)$$

where E is considered a function of the variables k. Substitution of (2.4) in (2.3) gives the Schrödinger equation of interaction representation

$$\left.\begin{aligned} & i\hbar(\partial/\partial t)\langle k \mid \psi(t) \\ &= \int \langle k \mid V \mid k' \rangle \exp[(E' - E)\, t/i\hbar]\; dk' \langle k' \mid \psi(t) \end{aligned}\right\} \qquad (2.5)$$

or, symbolically,

$$i\hbar\, \partial \psi(t)/\partial t = V(t)\psi(t) \qquad (2.6)$$

with $V(t)$ derived from V by the definition (1.19).

While in many cases it is useful to treat the system as if it were not closed and to have V itself depend on time (see Chapter IX), we shall now first assume that the system is closed and that the factor $\exp(E_{RL}t/i\hbar)$ of (1.19) constitutes the only time-dependence of $V(t)$. In that case, there are stationary states (labeled by n) for which

$$\psi_{Sn}(t) = \psi_{Sn} \exp(H_n t/i\hbar), \qquad (2.7)$$

so that, by (2.4),

$$\langle k \mid \psi_n(t) = \langle k \mid \psi \mid n \rangle \exp[(H_n - E)t/i\hbar)], \qquad (2.8)$$

where the time-independent coefficients $\langle k \mid \psi \mid n \rangle$ are the time-independent wave functions—eigenfunctions of H—in k-space.

In Dirac fashion we have inserted the label n in a "ket"; the matrix $\langle k \mid \psi \mid n \rangle$ has rows and columns labeled by different sets of variables; and the fact that there is a complete orthonormal set of eigenfunctions of H may be expressed by

$$\int \langle n \mid \psi^\dagger \mid k \rangle\, dk \langle k \mid \psi \mid n' \rangle = \langle n \mid n' \rangle, \qquad (2.9)$$
(orthonormality)

$$\int \langle k \mid \psi \mid n \rangle\, dn \langle n \mid \psi^\dagger \mid k' \rangle = \langle k \mid k' \rangle, \qquad (2.10)$$
(completeness)

or, symbolically, by

$$\psi^\dagger \psi = \mathbf{1}, \qquad \psi\psi^\dagger = 1. \tag{2.11}$$

We shall subdivide the time-independent wave functions into two groups:

(1) Those stationary state eigenfunctions which vanish rapidly for infinite separation of the particles in our system. Such eigenfunctions we call $\langle k \mid \psi_r$ or briefly ψ_r; they correspond to "bound states". They include states in which only part of the system is properly bound, while other particles are going off to infinity (see also Chapter IV).

(2) The remainder of the eigenfunctions $\langle k \mid \psi \mid n \rangle$, in general no longer a complete set of functions. They are the stationary states that are considered in such scattering problems, where all the particles are free after the scattering process. We shall call them "scattering states".

There are various methods for bringing some order in the scattering states. As asymptotically—for infinite separation of the particles—the scattering states satisfy the free-particle Schrödinger equation, one may first, crudely, represent them by a definite free-particle state labeled by the value k_0 of the variables in k-space. However, such free-particle state $\langle k \mid k_0 \rangle$ is of course no exact solution of the time-independent Schrödinger equation which, on account of (2.5) with (2.8), reads

$$(H_n - E) \langle k \mid \psi \mid n \rangle = \int \langle k \mid V \mid k' \rangle \, dk' \, \langle k' \mid \psi \mid n \rangle. \tag{2.12}$$

The scattering state with a plane wave part which asymptotically behaves like $\langle k \mid k_0 \rangle$ must correspond to a total energy $H_n = E_0$. If we succeed in further specifying the scattering state we have in mind, we use from then on k_0 as label of this scattering state. This further specification can be given in many different ways, each giving the scattering state labeled by k_0 a different meaning. Some of the most interesting possibilities are:

(a) By k_0 we denote a scattering state which asymptotically is a superposition of the free-particle state k_0 and of outgoing scattered waves. (By "outgoing" we mean that in xyz-space the scattered wave gives in a given direction (ϑ, φ) asymptotically

($r \to \infty$) for each scattered particle a probability density depending on the scattered wave in k-space for momentum of such particle in that same direction (ϑ, φ), but not depending on the scattered wave for momentum in the opposite direction).
(b) Or, by k_0 we might denote a scattering state which asymptotically is a superposition of the free state k_0 and of incoming additional waves.
(c) Or, by k_0 we could denote a scattering state which besides the free state k_0 asymptotically contains incoming and outgoing waves in some symmetric way.

The scattering state satisfying the description (a) we shall denote by $\langle k \mid \Psi \mid k_0 \rangle$, a scattering state of type (b) we shall call $\langle k \mid \Omega \mid k_0 \rangle$, and one of the kind described under (c) we shall call $\langle k \mid Q \mid k_0 \rangle$. Let $\langle k \mid Y \mid k_0 \rangle$ mean any of these three types of scattering states, specification still to be given. When k_0 takes all possible values, Ψ, Ω, Q, and Y become matrices in k-spaces, the scattering matrices. Ψ is identical with the "wave matrix" introduced in reference 4. Contrary to ψ, both labels are now values of the same set of variables k, but the scattering states do no longer form a complete orthonormal set and therefore Ψ, Ω, Q need not satisfy relations like (2.9)—(2.11); consequently, Ψ, Ω, Q in general are no unitary matrices. Still we can be sure that scattering states belonging to two different energy levels will be orthogonal.

On account of $H_n = E_0$, the Schrödinger equation (2.12) for the scattering states $\langle k \mid Y \mid k_0 \rangle$ may be written symbolically as

$$(E_R - E_L)\, Y = VY. \tag{2.13}$$

Since $\langle k \mid k_0 \rangle$—the unit matrix 1 in k-space—forms an essential part of the scattering states, we write (see Appendix C)

$$Y = 1 + Z, \tag{2.14}$$

so that, by

$$(E_R - E_L) \langle k_L \mid k_R \rangle = 0 \tag{2.15}$$

(2.13) gives

$$(E_R - E_L)\, Z = VY = V + VZ. \tag{2.16}$$

Further, we define

$$B \equiv VY, \tag{2.17}$$

so that the Schrödinger equation is reduced to two equations for two unknown matrices B and Z:

$$(E_R - E_L)\, Z = B; \tag{2.18}$$

$$V + VZ = B. \tag{2.19}$$

While elimination of B leads back to (2.16) and (2.13), we could eliminate Z by solving for it from (2.18). This gives

$$Z = ?\, B \,\|. \tag{2.20}$$

The uncertainty in the meaning of Y at the beginning is here expressed by the uncertainty of the meaning of the slash in (2.20).

The question therefore arises, which meaning of the slash in (2.20) corresponds to each of the interpretations (a), (b) or (c) of the set of scattering states $\langle k \,|\, Y \,|\, k_0 \rangle$. The answer is well known and is independent of the possibility of expansion. It can be shown[9), 4)] that

$$\S B \,\| = -2\,\pi\, i\, \delta_+ (E_{RL})\, B = \left\{ P(1/E_{RL}) - \pi\, i\, \delta (E_{RL}) \right\} B \tag{2.21}$$

is the only expression of the form (2.20) corresponding to outgoing waves only.

$$\flat\, B \,\| = \left\{ P\,(1/E_{RL}) + \pi\, i\, \delta\,(E_{RL}) \right\} B \tag{2.22}$$

is the only expression of the form (2.20) corresponding to incoming waves only, and both $'B \,\|$ and $_\delta B \,\|$ describe waves half incoming and half outgoing, but of these two only $'B \,\|$ has the form (2.20).

The general validity of the above statement, that a combination of the free particle state k_0 with outgoing waves only is the solution of (2.19)—(2.20) with $? = \S$, will become much clearer by the time-dependent methods discussed in Chapters V and VI.

We shall now separately discuss the three cases (a), (b), and (c). In case (a), we shall denote Y, Z, and B by Ψ, T, and F, respectively. In case (b), we shall denote them by Ω, Γ, and G. In case (c), we shall denote them by Q, P, and W. Thus, Eqs. (2.14), (2.20) and (2.17), (2.19) will in these three cases be read as

$$\Psi = 1 + T\,; \quad \Omega = 1 + \Gamma\,; \quad Q = 1 + P; \tag{2.23a-c}$$

$$T = \S\, F \| \quad ; \quad \Gamma = \flat\, G \| \quad ; \quad P = {}'W \|; \tag{2.24a-c}$$

$$\left.\begin{aligned} F = V\,\Psi = V + VT; \quad G = V\,\Omega = V + V\,\Gamma; \\ W = VQ = V + VP. \end{aligned}\right\} \tag{2.25a-c}$$

Substituting (2.20) with (2.17) into (2.14) we also find

$$Y = 1 + ?\, VY \|, \tag{2.26}$$

thence,

$$\left.\begin{aligned} \Psi = 1 + \S\, V\,\Psi \| \,; \quad \Omega = 1 + \flat\, V\,\Omega \|; \\ Q = 1 + {}'VQ \|. \end{aligned}\right\} \tag{2.27a-c}$$

Our definitions (2.23a)—(2.25a) of Ψ, T, and F are equivalent with Eqs. (10), (11) and (15) in reference 4, where we have defined HEISENBERG's characteristic S-matrix by Eqs. (23) and (26). In our present notation, these equations read

$$R = 2\,\delta F \| \,; \quad S = 1 + R. \tag{2.28}$$

Besides the quantity R expressible in terms of the wave matrix Ψ, we define an analogous quantity $-iK$, expressible in terms of the matrix Q, by

$$K = 2\,i\,\delta W \|. \tag{2.29}$$

Since $V = V^\dagger$ is Hermitian, (2.17) and the Hermitian conjugate of (2.17) read

$$B = VY, \; B^\dagger = Y^\dagger V. \tag{2.30}$$

Hence, for any of our interpretations of the slash we get

$$Y^\dagger B - B^\dagger Y = 0, \tag{2.31}$$

and for any pair of interpretations

$$Y_1^\dagger B_2 - B_1^\dagger Y_2 = 0. \tag{2.32}$$

From the three equations (2.31), which, by (2.23)—(2.25), may be written

$$\left.\begin{aligned} F - F^\dagger + T^\dagger F - F^\dagger T &= 0, \quad \text{a)} \\ G - G^\dagger + \Gamma^\dagger G - G^\dagger \Gamma &= 0, \quad \text{b)} \\ W - W^\dagger + P^\dagger W - W^\dagger P &= 0, \quad \text{c)} \end{aligned}\right\} \tag{2.33}$$

one easily derives the following equations

$$\left.\begin{aligned} \Psi^\dagger \Psi &= 1, \quad \text{a)} \\ \Omega^\dagger \Omega &= 1, \quad \text{b)} \\ Q^\dagger Q &= 1 + \left(\frac{K}{2}\right)^2. \quad \text{c)} \end{aligned}\right\} \tag{2.34}$$

We shall give a detailed proof of the last equation only, the proof of the two other equations (2.34) running in the same way. First we get from (2.33c), by multiplication with $2\pi\delta(E_{RL})$,

$$2i\delta W\| - 2i\delta W^\dagger\| + 2i\| W^\dagger{}' W\delta - 2i\delta W^\dagger{}' W\| = 0, \tag{2.35}$$

where we have used (2.24c) and one of the rules (1.7). Further, on account of these rules, the two last terms on the left-hand side of this equation cancel and $\delta W^\dagger\| = -(\delta W\|)^\dagger$, so that (2.35) gives

$$K = K^\dagger, \tag{2.36}$$

which shows that K as defined by (2.29) is Hermitian. Further, multiplying (2.33c) by $D_{RL} = -D_{LR}$ we get, by means of (2.24c) and (1.7),

$$'W\| - 'W^\dagger\| - \| W^\dagger{}' W' - 'W^\dagger{}' W\| = 0. \tag{2.37}$$

Using the fundamental relation (1.18), the third and fourth term in this equation give

$$\left.\begin{aligned} &{}'W^\dagger \,\|\, W' + {}_\delta W^\dagger \,\|\, W_\delta \\ &= (\|\, W^{\dagger\prime}) \cdot ({}'W\|) + (\|\, W^\dagger{}_\delta) \cdot ({}_\delta W\|) = P^\dagger P - \left(\frac{K}{2}\right)^2, \end{aligned}\right\} \quad (2.38)$$

where we have used the definitions (2.24c) and (2.29) of P and K and the general rules (1.7) for taking the Hermitian conjugates of these quantities.

Thence, (2.37) gives

$$P + P^\dagger + P^\dagger P - K^2/4 = 0$$

or

$$Q^\dagger Q = (1 + P^\dagger)(1 + P) = 1 + K^2/4,$$

i. e. (2.34c). The equations (2.34, a, b) may be proved along similar lines by multiplying (2.33, a, b) by $(E_{RL} + ia)^{-1} = -(E_{LR} - ia)^{-1}$ and using the important relation

$$\|\, A \natural B \natural + \S A \,\|\, B \natural + \S B \,\| = 0, \quad (1.18a)$$

which follows from (1.18) by (1.9) and (1.7).

The equation (2.34a) is identical with Eq. (62) in reference 4, but the proof given there was not quite satisfactory.

Like (2.9) or the first equation (2.11), Eq. (2.34 a) expresses the orthonormality of the scattering states $\langle k \,|\, \Psi \,|\, k_0 \rangle$; but the unit matrix $1 = \langle k_L \,|\, k_R \rangle$ occurring in this equation is only a submatrix of the unit matrix $\mathbf{1} = \langle n_L \,|\, n_R \rangle$ of (2.9)—(2.11) and one has to add to the stationary states $\langle k \,|\, \Psi \,|\, k_0 \rangle$ the bound states $\langle k \,|\, \psi_r$ in order to form a complete set of functions. (This under the supposition that the $\langle k \,|\, \Psi \,|\, k_0 \rangle$ form at least a complete set of scattering states). Then, Eq. (2.10) may be written as

$$\left.\begin{aligned} &\int \langle k \,|\, \Psi \,|\, k_0 \rangle \, dk_0 \langle k_0 \,|\, \Psi^\dagger \,|\, k' \rangle + \sum_r \langle k \,|\, \psi_r) \cdot (\psi_r^\dagger \,|\, k' \rangle \\ &\qquad = \langle k \,|\, k' \rangle \end{aligned}\right\} \quad (2.39)$$

or, symbolically[4],

$$\Psi\Psi^\dagger = 1 - \sum_r \psi_r \cdot \psi_r^\dagger, \tag{2.40}$$

where we have introduced the bound state matrices ψ_r, $\psi_r^\dagger$ with only one column and one row, respectively. This shows that Ψ cannot be unitary if there are bound states.

For the three different pairs of interpretations of the slash, the equations (2.32) take the form

$$\left.\begin{aligned} &\Psi^\dagger G - F^\dagger \Omega = 0, \text{ i. e. } G - F^\dagger + T^\dagger G - F^\dagger \Gamma = 0, && \alpha) \\ &\Psi^\dagger W - F^\dagger Q = 0, \text{ i. e. } W - F^\dagger + T^\dagger W - F^\dagger P = 0, && \beta) \\ &\Omega^\dagger W - G^\dagger Q = 0, \text{ i. e. } W - G^\dagger + \Gamma^\dagger W - G^\dagger P = 0. && \gamma) \end{aligned}\right\} \tag{2.41}$$

By multiplying (2.41, β) by $-2\pi i \delta(E_{RL})$, we find

$$\begin{aligned} 0 &= 2\,\delta W \| - 2\,\delta F^\dagger \| + 2 \| F^\dagger \flat W_\delta - 2\,\delta F^\dagger {}' W \| \\ &= 2\,\delta W \| + 2\,(\delta F \|)^\dagger + 2\,\delta F^\dagger (\flat - ') W \| \\ &= -iK + R^\dagger - \frac{1}{2} i R^\dagger K, \end{aligned}$$

where we have used the definitions of T, P, K and R along with the rules (1.7) and (1.9). The Hermitian conjugate of this equation is

$$\left(1 + \frac{1}{2} iK\right) R = -iK. \tag{2.42}$$

In this way, we have obtained Heitler's integral equation [7) 8)] without the use of series expansions.

Since K is Hermitian, all the eigenvalues of the matrix $1 + \frac{iK}{2}$ are different from zero. Thus, this matrix has a reciprocal $\left(1 + \frac{iK}{2}\right)^{-1}$, and (2.42) gives

$$R = \frac{-iK}{1 + \frac{iK}{2}}. \tag{2.43}$$

For the S-matrix (2.28) we thus get

$$S = 1 + R = \frac{1 - iK/2}{1 + iK/2} \tag{2.44}$$

in terms of the "reaction operator" K (comp. Eq. (1.34) of reference 1).

In this form, the unitarity of the S-matrix is obvious, viz.

$$S^\dagger S = SS^\dagger = 1. \tag{2.45}$$

Multiplying (2.41 α) by $-2\pi i\,\delta(E_{RL})$ we find that the two last terms in the left-hand member cancel and we get

$$R_- \equiv 2\,\delta G\| = -2\,(\delta F\|)^\dagger = -R^\dagger. \tag{2.46}$$

Multiplication of the Eqs. (2.33 a, b) and (2.41 γ) by $-\pi i\,\delta(E_{RL})$ does not lead to new information. In fact, the equations obtained in this way are, on account of Eq. (2.46), equivalent with the equations (2.45) and (2.43).

However, by multiplying the Eqs. (2.41) by $(E_{RL} + ia)^{-1} = -(E_{LR} - ia)^{-1}$, we get by (1.18), by a similar procedure as that used in deriving (2.34) from (2.33),

$$\left.\begin{aligned} \Psi^\dagger \Omega &= S^\dagger, && \alpha) \\ \Psi^\dagger Q &= 1 + \frac{iK}{2}, && \beta) \\ \Omega^\dagger Q &= 1 - \frac{iK}{2}. && \gamma) \end{aligned}\right\} \tag{2.47}$$

These equations determine the connection between the three different types of scattering states Y denoted by Ψ, Ω, and Q. We have assumed above that the set of functions $\langle k \mid \Psi \mid k_0 \rangle$ forms a complete set of *scattering* states. We shall make the same assumption about the set of functions $\langle k \mid Y \mid k_0 \rangle$. Whenever these assumptions are justified, any function expressible as a superposition of scattering states $\langle k \mid \Psi \mid k_0 \rangle$ can also be expressed as a superposition of scattering states $\langle k \mid \Omega \mid k_0 \rangle$ *or*

$\langle k \mid Q \mid k_0 \rangle$, and vice versa. Therefore, matrices X_1 and X_2 must exist, such that

$$\Omega = \Psi X_1, \quad Q = \Psi X_2.$$

From (2.47) and (2.34 a) we then get

$$X_1 = S^\dagger, \quad X_2 = 1 + \frac{iK}{2},$$

i. e. (see Appendix D)

$$\Psi = \Omega S = Q\left(1 + \frac{iK}{2}\right)^{-1}, \tag{2.48}$$

where we have used the unitarity of the S-matrix. With (2.48) the equations (2.47), (2.34, b, c) are easily seen to be consequences of the Eq. $\Psi^\dagger \Psi = 1$. From (2.48) we see that the scattering state matrix Ψ, corresponding to outgoing waves only, is obtained from the matrix Ω corresponding to ingoing waves by multiplication on the right with the S-matrix.

If we define a matrix δ by

$$K = -2 \tan \delta, \tag{2.49}$$

we have, on account of (2.44),

$$S = \frac{1 + i \tan \delta}{1 - i \tan \delta} = \frac{e^{i\delta}}{e^{-i\delta}} = e^{i2\delta} = e^{i\eta}, \tag{2.50}$$

where

$$\eta = 2\delta \tag{2.51}$$

is the Hermitian η-matrix introduced by HEISENBERG. In the simple case of a scattering of particles by a fixed potential in configuration space, the eigenvalues δ' of the matrix δ are the "phase shifts" of the scattered waves.[1) 2)]

III. Time-independent perturbation treatment.

We shall now try to solve the time-independent Schrödinger equation (2.13) or (2.19)—(2.20) for the scattering states by a series expansion in the potential V, starting from $Y \approx 1$. Series expansions of any quantity like Y, Z, B, etc. will be denoted by a subscript asterisk, i. e. by Y_*, Z_*, B_*, etc. It is seen by inspection that the series

$$\left.\begin{aligned} B_* &= \sum_{n=1}^{\infty} V(?V)^{n-1}\,\| = \sum_{n=1}^{\infty} V\underbrace{(?V?V?V\cdots?V)}_{n-1 \text{ factors}}\,\| \\ Z_* &= \sum_{n=1}^{\infty} (?V)^n\,\| = \sum_{n=1}^{\infty} \underbrace{?V?V\cdots?V}_{n \text{ factors}}\,\| \end{aligned}\right\} \tag{3.1}$$

solve the equations (2.19)—(2.20) whenever these expansions converge; and if one assumes that it should be possible to find B and Z from (2.19)—(2.20) by successive approximations starting from $Z \approx 0$, it is easily seen that (3.1) is the only solution. Thus, if the series converge,

$$Y_* = 1 + Z_* = \sum_{n=0}^{\infty} (?V)^n\,\| \tag{3.2}$$

is the solution of (2.26) and represents a scattering state. With the three different meanings of the slash, we thus get for the scattering states (a), (b), and (c)

$$\Psi_* = \sum_{n=0}^{\infty} (\S V)^n\,\|;\ T_* = \sum_{n=1}^{\infty} (\S V)^n\,\|;\ F_* = \sum_{n=1}^{\infty} V(\S V)^{n-1}\,\|, \tag{3.3a}$$

$$\Omega_* = \sum_{n=0}^{\infty} (\flat V)^n\,\|;\ \Gamma_* = \sum_{n=1}^{\infty} (\flat V)^n\,\|;\ G_* = \sum_{n=1}^{\infty} V(\flat V)^{n-1}\,\|, \tag{3.3b}$$

$$Q_* = \sum_{n=0}^{\infty} ('V)^n\,\|;\ P_* = \sum_{n=1}^{\infty} ('V)^n\,\|;\ W_* = \sum_{n=1}^{\infty} V('V)^{n-1}\,\|. \tag{3.3c}$$

For the matrices R, K and S, defined by (2.28)—(2.29), we then get the following series expansions:

$$R_* = 2\sum_{n=1}^{\infty}{}_{\delta}V(\S V)^{n-1}\|, \tag{3.4}$$

$$K_* = 2i\sum_{n=1}^{\infty}{}_{\delta}V('V)^{n-1}\|, \tag{3.5}$$

$$S_* = 1 + 2\sum_{n=1}^{\infty}{}_{\delta}V(\S V)^{n-1}\|. \tag{3.6}$$

The expression (3.5) for K_* shows directly that K_* is Hermitian in accordance with (2.36). In fact, we have, according to the general rules (1.7)—(1.8),

$$\left.\begin{aligned} K_*^{\dagger} &= 2i\sum_{n=1}^{\infty}\|('V)^{n-1}V_{\delta} = 2i\sum_{n=1}^{\infty}{}_{\delta}('V)^{n-1}V\| \\ &= 2i\sum_{n=1}^{\infty}{}_{\delta}V('V)^{n-1}\| = K_*. \end{aligned}\right\} \tag{3.7}$$

By direct multiplication of the series it is easily seen that the orthogonality conditions (2.34) are satisfied by the expressions (3.3) (see Appendix B). It would now be interesting also to calculate $\Psi_*\Psi_*^{\dagger}$ in order to get some information about the bound states through (2.40). Since

$$\Psi_* = \sum_{n=0}^{\infty}(\S V)^n\|; \quad \Psi_*^{\dagger} = \sum_{n=0}^{\infty}\|(V\flat)^n, \tag{3.7}$$

we get by multiplication of the series

$$\left.\begin{aligned} \Psi_*\Psi_*^{\dagger} &= \sum_{i,j=0}^{\infty}(\S V)^i\|(V\flat)^j \\ &= \sum_{n=0}^{\infty}\left(\sum_{l=0}^{n}(\S V)^l\|(V\flat)^{n-l}\right) \equiv \sum_{n=0}^{\infty}A_n. \end{aligned}\right\} \tag{3.8}$$

From the definitions of scat and flat we get

$$\left.\begin{aligned} &A_0 = 1; \qquad A_1 = \S V\| + \|V\flat = 0; \qquad \langle k_0|A_n|k_n\rangle \\ &= \int\langle k_0|V|k_1\rangle dk_1\langle k_1|V|k_2\rangle\cdots dk_{n-1}\langle k_{n-1}|V|k_n\rangle B(n), \end{aligned}\right\} \tag{3.9}$$

$$B(n) = \sum_{l=0}^{n} \prod_{i=0}^{l-1} (E_l - E_i + ia)^{-1} \prod_{j=l+1}^{n} (E_l - E_j - ia)^{-1} \text{ for } n \geqslant 2, \quad (3.10)$$

where $\prod_{i=0}^{-1} (E_0 - E_i + ia)^{-1}$ and $\prod_{j=n+1}^{n} (E_n - E_j - ia)^{-1}$ both mean 1.

In Appendix B, it is shown that all $B(n)$ contain a as a factor, so that $A_n \to 0$ when the limit $a \to 0$ is taken after the integration in (3.9). Hence,

$$\left.\begin{aligned} A_n &= 0 \quad \text{for} \quad n \geqslant 1 \\ \text{and} \qquad & \\ \Psi_* \Psi_*^\dagger &= 1, \end{aligned}\right\} \quad (3.11)$$

i. e. Ψ_* has $\Psi_*^\dagger$ as its inverse, and therefore is unitary.

By comparison with the exact equation (2.40) this is seen to be possible only if the system has no bound states. We therefore have come to the interesting conclusion *that the series expansions (3.3) of the scattering state matrices must diverge whenever the system has bound states,* even if the coupling constants entering in V are small. This, of course, does not mean that the series expansion of every scattering wave function $\langle k \mid \Psi \mid k_0 \rangle$ will diverge for a system with bound states; it only means that the series $\langle k \mid \Psi_* \mid k_0 \rangle$ cannot be convergent for all k_0. It also does not necessarily mean that the expansion (3.6) of the S-matrix diverges, since S is unitary also when the system has bound states. Our result merely shows that no information about possible bound states of the system can be obtained by a perturbation treatment.

If the series converge, the Eqs. (2.48) are easily verified by direct multiplication of the series. Take, for instance, the equation

$$\Psi_* = Q_* \left(1 + \frac{iK_*}{2}\right)^{-1} = Q_* \sum_{n=0}^{\infty} \left(\frac{K_*}{2i}\right)^n. \quad (3.12)$$

By (3.5) and by use of the rules (1.7), (1.9) the right-hand member of (3.12) is

$$\sum_{n=0}^{\infty} \left[\sum_{i=0}^{\infty} (' V)^i\right] \left[\delta V \sum_{j=0}^{\infty} (' V)^j\right]^n \Bigg\|, \quad (3.13)$$

while the left-hand member may be written

$$\Psi_* = \sum_{p=0}^{\infty} ('V + \delta V)^p \Big\| . \tag{3.14}$$

The equality of (3.13) and (3.14) is obvious if we may change orders of sequence of summations, as both (3.13) and (3.14) represent summations over terms containing arbitrary numbers of $('V)$-factors, with arbitrary numbers of (δV)-factors interspersed at arbitrary positions.

Finally note that, if the expansion in (3.12) converges, not only Ψ_* has an inverse $\Psi_*^\dagger$, but also Q_* has an inverse

$$Q_*^{-1} = \sum_{n=0}^{\infty} \left(-\frac{1}{2} iK_*\right)^n \Psi_*^\dagger . \tag{3.15}$$

Also, by (2.45), (2.48), and (2.34a) with (3.11), $\Omega_*^\dagger = S_* \Psi_*^\dagger$ is then the inverse of $\Omega_* = \Psi_* S_*$.

IV. Interpretation of the scattering matrix Ψ and of the characteristic matrix S.

The scattering state $\langle k \mid \Psi \mid k_o \rangle$ obviously can be interpreted as representing incident particles in free-particle state k_0, and scattered particles described by the asymptotic behaviour of the (outgoing) wave $\langle k \mid T \mid k_o \rangle$. (Absorption from the incident beam is described by interference of incident and scattered waves). Values for differential cross sections follow directly from such interpretation. (See section 2 of reference 4). They are found by calculating the value of the probability density for one of the scattered particles for large radial distance in a given direction in xyz-space, and are found to be proportional to the absolute square of the matrix element of the "effective scattering potential" F for a transition to a final state, in which the momentum of the particle considered is directed in the direction into which the scattering probability of that particle was to be calculated and has the magnitude corresponding to energy conservation.

Since

$$F\big|_{E_{RL}=0} = \frac{i}{2\pi}\int_{-}^{+}(S-1)\,dE_{RL}, \qquad (4.1)$$

the cross sections for processes in which all the particles are free after the collision are uniquely determined by the matrix elements of the S-matrix. It should be noted, however, that the S-matrix and the wave matrix Ψ defined in II and in references 2 and 4 do *not* account for collision processes in which part of a system is in a bound state before and after the collision. This follows at once from the fact that the function

$$\langle x \,|\, \Psi \,|\, k_0 \rangle = \int \langle x \,|\, k \rangle \, dk \, \langle k \,|\, \Psi \,|\, k_0 \rangle$$

in configuration space represents plane waves superimposed by outgoing waves for *all* the particles. Such processes must therefore be described by state functions ψ_r which belong to the group of states classified as "bound states" in II.

On the other hand, it is clear that we could have started from a different division of the total Hamiltonian in (2.3). We could, for instance, let E denote the total Hamiltonian of a part of the total system plus the free particle energy of the rest of the system, while V is the rest of the potential not included in E. If k now is a set of variables commuting with each other and with this new operator E, we could formally proceed in the same way as in the preceding chapters, using a kind of "partial" interaction representation with the Schrödinger equation (2.6), but with a different interpretation of the quantities occurring in the equation. Also the division into "scattering" states and bound states would be different in such a treatment, and we would arrive at an S-matrix or a "collision" matrix which in general is not simply a different representation of the Heisenberg S-matrix. Such a procedure is often used in the treatment of collisions between elementary particles and atomic nuclei. To each division of the total Hamiltonian in (2.3) we get in this way a corresponding S-matrix, and the connection between these collision matrices is not always simple. Throughout this paper, we shall explicitly consider only the case where E is the free particle energy, but

our considerations can easily be extended to the case where E includes part of the interaction.

Since

$$S = 1 + 2\,\delta F\| = 1 + \S\, F\| - \flat\, F\| = 1 + R, \qquad (4.2)$$

$$\Psi = 1 + \S\, F\| = 1 + T, \qquad (4.3)$$

we get

$$R = T - \flat\, F\|. \qquad (4.4)$$

While $T = \S\, F\|$ in xyz-space asymptotically represents outgoing waves only[2),4)] $\flat\, F\|$ represents incoming waves only. Hence, while $\langle k \,|\, \Psi \,|\, k_0 \rangle$ gives a correct direct picture of the scattering phenomenon as it represents a superposition of a plane wave with spherical outgoing waves only, on the other hand $\langle k \,|\, S \,|\, k_0 \rangle$ represents in k-space a superposition of a plane wave with an incoming and an outgoing spherical wave. This gives rise to a paradox to which we shall come back in the discussion of the time-dependent wave function for $t \to \infty$ (see Chapter VII).

V. Time-dependent scattering theory and Dyson's S-matrix.

Use of time-dependent methods in scattering theory is based on a simple idea: "If very long ago (formally: "in the infinite past, at $t = -\infty$") there were only particles in the initial free-particle state k_0, then by now this non-stationary state will have developed into the corresponding stationary scattering state". Often one adds to this the remark that, if one for establishment of this scattering state waits from $t = -\infty$ to $t =$ finite, one may as well wait till $t = +\infty$ and consider scattering as a process taking place between $t = -\infty$ and $t = +\infty$.

We start by solving the Schrödinger equation (2.6) for the wave-function $\psi(t)$ in interaction representation systematically. As boundary condition, let $\psi(t_0)$ be given. The linear relation between $\psi(t)$ and $\psi(t_0)$ we express by means of the "propagation matrix" $U(t, t_0)$ as follows:

$$\langle k \,|\, \psi(t) = \int \langle k \,|\, U(t, t_0) \,|\, k' \rangle \, dk' \, \langle k' \,|\, \psi(t_0) \qquad (5.1)$$

or, briefly,

$$\psi(t) = U(t, t_0)\, \psi(t_0). \qquad (5.2)$$

As we assume that the Schrödinger equation (2.6) may be used to find $\psi(t + dt)$ from $\psi(t)$ for $dt < 0$ as well as for $dt > 0$,* we may also interchange t and t_0 in (5.2). Thence,

$$\psi(t) = U(t, t_0)\, U(t_0, t)\, \psi(t), \qquad (5.3\,a)$$

$$U(t_0, t) = U(t, t_0)^{-1}, \qquad (5.3\,b)$$

that is, the propagation matrix U has a reciprocal.

Substituting (5.2) into (2.6) we find

$$\left.\begin{aligned} i\hbar\, \partial\, U(t, t_0) / \partial\, t &= V(t)\, U(t, t_0) \\ &= \{ V \exp(E_{RL} t / i\hbar \} \, U(t, t_0), \end{aligned}\right\} \qquad (5.4)$$

where $V = V^{\dagger}$, and by (1.21)

$$V(t)^{\dagger} = V(t).$$

Let $\langle k \,|\, \psi(t) \,|\, n \rangle$ or, briefly, $\psi_n(t)$ form a set of solutions of the Schrödinger equation (2.6), complete and orthonormal at a given time t_0; that is, the relations

$$\left.\begin{aligned} &\int \langle n' \,|\, \psi^{\dagger}(t) \,|\, k \rangle \, dk \langle k \,|\, \psi(t) \,|\, n \rangle = \langle n' \,|\, n \rangle \\ \text{or} \quad &\psi^{\dagger}_{n'}(t)\, \psi_n(t) = \langle n' \,|\, n \rangle \quad \text{or} \quad \psi^{\dagger}(t)\, \psi(t) = \mathbf{1} \end{aligned}\right\} \qquad (5.5)$$

and

$$\sum_n \langle k \,|\, \psi(t) \,|\, n \rangle \langle n \,|\, \psi^{\dagger}(t) \,|\, k' \rangle = \langle k \,|\, k' \rangle$$

or

$$\sum_n \psi_n(t)\, \psi^{\dagger}_n(t) = 1 \quad \text{or} \quad \psi(t)\, \psi^{\dagger}(t) = 1 \qquad (5.6)$$

* In "integrocausal" theories, such assumption may be dropped[10].

are valid at $t = t_0$. We shall now first prove conservation of orthonormality (5.5) even if V in (2.3) in Schrödinger representation depends on time, as for a non-closed system.

Eq. (5.5) can in symbolic notation be written by (5.2) as

$$\psi(t_0)^\dagger U(t, t_0)^\dagger U(t, t_0) \psi(t_0) = \mathbf{1}. \tag{5.7}$$

Now, by (5.2),

$$U(t_0, t_0) = 1 = U(t_0, t_0)^\dagger, \tag{5.8}$$

so that the equation

$$U(t, t_0)^\dagger U(t, t_0) = 1 \tag{5.9}$$

is trivial for $t = t_0$. As t becomes different from t_0, Eq. (5.9) remains valid, because

$$\left.\begin{aligned} & i\hbar(\partial/\partial t)\left\{U(t, t_0)^\dagger U(t, t_0)\right\} \\ = {} & U(t, t_0)^\dagger V(t) U(t, t_0) - \left\{V(t)\ U(t, t_0)\right\}^\dagger U(t, t_0) = 0. \end{aligned}\right\} \tag{5.10}$$

Thence, the left hand members of (5.5) and (5.7) equal $\psi(t_0)^\dagger \psi(t_0)$, which was given to be equal to $\mathbf{1} = \langle n' \mid n \rangle$.

We shall now prove that also (5.6) remains valid as t becomes different from t_0. Indeed, the left-hand member of (5.6) depends on time according to

$$\left.\begin{aligned} & i\hbar(\partial/\partial t)\left\{\psi(t)\psi(t)^\dagger\right\} \\ = {} & V(t)\psi(t)\psi(t)^\dagger - \psi(t)\psi(t)^\dagger V(t)^\dagger, \end{aligned}\right\} \tag{5.11}$$

so, whenever $\psi(t)\psi(t)^\dagger = 1$, we find its time derivative to be equal to $\left\{V(t) - V(t)^\dagger\right\}/i\hbar = 0$. Therefore, $\psi(t)\psi(t)^\dagger$, once equal to the unit matrix, will always remain the unit matrix, provided that $\psi(t)\psi^\dagger(t)$ is an analytic function of t.

Next, we shall show the unitarity of $U(t, t_0)$. Making use of the existence of a reciprocal (5.3b) of $U(t, t_0)$ we find, by (5.9),

$$UU^\dagger = UU^\dagger UU^{-1} = UU^{-1} = 1. \tag{5.12}$$

Thence, U is unitary, i. e.

$$U^\dagger = U^{-1} \tag{5.13}$$

is the reciprocal of U, and (5.3b) gives

$$U(t, t_0)^\dagger = U(t_0, t). \tag{5.14}$$

We shall now first consider the case of a closed system with V independent of time, so that $V(t)$ depends on time by the factor explicitly given in (1.19) only. Again we may distinguish stationary scattering states and bound states; in interaction representation, the latter depend on time by (2.6)—(2.8), or

$$i\hbar\,\partial\,\psi_r(t)/\partial\,t = (H_n - E_L)\,\psi_r(t) = V(t)\,\psi_r(t), \tag{5.15}$$

while the time-dependence of scattering states $Y(t)$ is given by (1.19), (2.6), (2.13):

$$i\hbar\,\partial\,Y(t)/\partial\,t = E_{RL}\,Y(t) = V(t)\,Y(t). \tag{5.16}$$

In Chapter II we assumed ψ_r and Ψ to form a complete orthonormal set of functions at $t = 0$; therefore, the solutions $\psi_r(t)$ and $\Psi(t)$ of (2.6) always form a complete orthonormal set, and Eqs. (5.5)—(5.6) may be written as

$$\left.\begin{aligned} &\Psi^\dagger(t)\,\Psi(t) = 1; && \Psi^\dagger(t)\,\psi_r(t) = 0, \\ &\psi_r^\dagger(t)\,\Psi(t) = 0; && \psi_{r'}^\dagger(t)\,\psi_r(t) = \delta_{r'r}, \end{aligned}\right\} \tag{5.17}$$

$$\Psi(t)\,\Psi^\dagger(t) + \sum_r \psi_r(t)\cdot\psi_r^\dagger(t) = \mathbf{1}, \tag{5.18}$$

where all matrices may now be taken time-dependent: $\psi_r(t)$ according to (2.8), and $\Psi(t)$ according to (1.19).

The Eqs. (5.4), (5.8) are now obviously solved by

$$\left.\begin{aligned} U(t, t_0) &= \Psi(t)\,\Psi^\dagger(t_0) + \sum_r \psi_r(t)\cdot\psi_r^\dagger(t_0) \\ &= \{\Psi \exp(E_{RL}\,t/i\hbar)\}\{\Psi^\dagger \exp(E_{RL}\,t_0/i\hbar)\} \\ &+ \sum_r \{\psi_r\cdot\psi_r^\dagger \exp[(E_R\,t_0 - H_r\,t_0 + H_r\,t - E_L\,t)/i\hbar]\}. \end{aligned}\right\} \tag{5.19}$$

Eq. (5.8) is satisfied on account of (5.18); Eq. (5.4) is satisfied on account of (5.15)—(5.16).

In fact, on account of Eqs. (5.17), Eq. (5.19) gives, for scattering states and for bound states, respectively,

$$\left.\begin{aligned} U(t, t_0)\, \Psi(t_0) &= \Psi(t), \quad \text{a)} \\ U(t, t_0)\, \psi_r(t_0) &= \psi_r(t). \quad \text{b)} \end{aligned}\right\} \tag{5.20}$$

We see that the propagation matrix $U(t, t_0)$ consists of two parts. The first part,

$$S(t, t_0) = \Psi(t)\, \Psi^\dagger(t_0), \tag{5.21}$$

changes a scattering state at time t_0 into one at time t, but destroys all bound-state admixtures in the wave function. The second part,

$$s(t, t_0) = \sum_r \psi_r(t)\, \psi_r^\dagger(t_0), \tag{5.22}$$

takes care of the propagation of bound-state wave functions.

From (1.22), applied to the matrices R, K, and S, which all contain a delt, we see that

$$R(t) = R, \quad K(t) = K, \quad S(t) = S \tag{5.23}$$

are constant in time. Hence, whenever (2.48) is valid (see Appendix D), Eqs. (5.19) and (5.21) may also be written

$$\left.\begin{aligned} U(t, t_0) &= S(t, t_0) + s(t, t_0), \quad \text{a)} \\ S(t, t_0) &= \Omega(t)\, \Omega^\dagger(t_0) = Q(t) \left[1 + \left(\frac{K}{2}\right)^2\right]^{-1} Q^\dagger(t_0), \quad \text{b)} \end{aligned}\right\} \tag{5.24}$$

where we have used the unitarity of S and the reality of K.

From (5.21), (5.24b), and (2.34a-c) it is seen that then also

$$S(t, t_0)\, \Psi(t_0) = \Psi(t); \quad S(t, t_0)\, \Omega(t_0) = \Omega(t);$$
$$S(t, t_0)\, Q(t_0) = Q(t),$$

so that $S(t, t_0)$ takes care of the propagation of the scattering states $\Omega(t)$ and $Q(t)$ as well as of the scattering states $\Psi(t)$.

We shall now consider the question of what becomes in course of time of a state given at $t_0 = -\infty$ and what happens to the wave function as $t \to +\infty$.

First, we shall formally define

$$U_+(t) = U(t, -\infty) = \lim_{t_0 \to -\infty} U(t, t_0), \tag{5.25a}$$

$$U_-(t) = U(t, +\infty) = \lim_{t_0 \to \infty} U(t, t_0); \tag{5.25b}$$

assuming that these limits exist.

Now, by (2.23a)—(2.24a) with (1.19) and (1.26), (1.27) with (2.28) we find

$$\text{“}\Psi(-\infty) = 1, \quad \Psi(+\infty) = 1 + 2\,{}_\delta F\| = S.\text{”} \tag{5.26}$$

Similarly, by (2.23b)—(2.24b), (1.28). (1.29), (2.46), and (2.28),

$$\text{“}\Omega(-\infty) = S^\dagger, \quad \Omega(+\infty) = 1.\text{”} \tag{5.27}$$

The second formula (5.26) and the first formula (5.27) require justification for the limit $t \to \pm\infty$ after the limit $a \to 0$, so that $a\,|\,t\,|$ remains small. This is justified, however, since we assumed no time-dependence of V at all, so that we need $a \to 0$ indeed to have (2.14)—(2.20) satisfy (2.13). Moreover, the first Eq. (5.27) follows from the first Eq. (5.26) and the second Eq. (5.26) follows from the second Eq. (5.27) by Eq. (2.48) whenever that one is valid.

As for the bound states, $\psi_r(\pm\infty)$ is somewhat meaningless. Formally, one may reason[5), 6)] that these expressions “vanish”:

$$\text{“}\psi_r(\pm\infty) = 0\text{”}. \tag{5.28}$$

(MA[6)] calls (5.28) a “conditional equality”.) If the convention (5.28) is accepted, we formally find, by (5.22), (5.24a), (5.25),

$$\text{“}s(t, \mp\infty) = 0\text{”}; \qquad \text{“}S(t, \mp\infty) = U_\pm(t).\text{”} \tag{5.29}$$

Thus, by (5.21) and (5.26),

$$\text{“}U_+(t) = \Psi(t)\,\Psi^\dagger(-\infty) = \Psi(t) = Q(t)\left(1 + \frac{iK}{2}\right)^{-1}\text{”} \tag{5.30a}$$

$$\left.\begin{aligned} ``U_-(t) &= \Psi(t)\,\Psi^\dagger(+\infty) = \Psi(t)\,S^{-1} = \Omega(t) \\ &= Q(t)\left(1-\frac{1}{2}\,iK\right)^{-1}", \end{aligned}\right\} \quad (5.30\,\mathrm{b})$$

where we have used (2.48), which holds also for the time-dependent quantities.

This should not be construed as to mean that, if at $t_0 = -\infty$ the wave function contains some bound state admixtures, then at finite time t such bound state should have died out; for, if $U(t)$ operates, say on $\psi_r(t_0 \to -\infty)$, the time dependence of the last factor $\psi_r^\dagger(t_0)$ in $U(t, t_0)$ apparently cancels the time dependence in the wave function $\psi_r(t_0)$ on which U operates, and the limit (5.28) should not be used. That is, while on account of conditional equalities we have "$\psi_r(-\infty) = 0$" as well as "$\psi_r^\dagger(-\infty) = 0$", yet $\lim_{t\to-\infty} \psi_r(t)^\dagger\,\psi_r(t) \neq 0$. Therefore, use of (5.28)—(5.30) should always be made with caution.

DYSON[3] defines the S-matrix as $U_+(+\infty)$. In fact, (5.30 a) with (5.26) and (5.29) gives

$$``S(\infty, -\infty) = U_+(\infty) = \Psi(\infty) = S", \qquad (5.31)$$

so that DYSON's definition is in agreement with the definition of HEISENBERG's characteristic matrix in references 2 and 4, as far as (5.28)—(5.30) are justified, that is, as long as this matrix is applied to scattering states only.

In this connection, it should be noted that the limits (5.26) too are only "conditional equalities"; in fact, their validity is closely related to (5.28). For, if (5.26) is true, then $\langle k \,|\, \Psi(-\infty) \,|\, k_0\rangle = \langle k \,|\, k_0\rangle$, that is, at $t = -\infty$, the scattering functions in k-space (labeled by k_0) form by themselves a complete set of functions (the free-particle states k_0); and, since all bound states were to be orthogonal to all scattering states, there could be no bound states at $t = -\infty$. That is, our possibility of writing (5.26) is based on granting the validity of (5.28)—(5.29).

On the other hand, when we meet the necessity of considering wave functions with bound state admixtures, so that we want to drop Eqs. (5.28)—(5.29) for them, then we should also drop Eq. (5.26), thence Eqs. (5.30)—(5.31). In that case, we have a

choice between either completely abandoning the use of interaction representation and using Heisenberg representation, where there are no such difficulties, or we shall have to settle on use of the more complicated Eq. (5.19) instead of the idealization which is the S-matrix, for predicting future states from past states.

We conclude that, as far as the foregoing treatment of the Dyson S-matrix is meaningful at all, we have

$$\text{“}\Psi(-\infty)\,\Psi(-\infty)^{\dagger} = 1\text{”}, \tag{5.32}$$

so that, by (2.34a) and (5.32), $\Psi(-\infty)$ is unitary. Also, to the same extent, $\Psi(+\infty)$ is unitary, by (5.26) with (2.45). Yet, $\Psi(t)$ is not unitary for intermediate values of t, on account of (5.18).

In justifying (5.28)—(5.29), MA[6] excluded the common case that, in $\langle k \mid \psi_r(t)$, E might equal H_r. It may be reasoned that (5.28) is still conditionally valid as long as $\langle k \mid \psi_r$ has no irregularities at $E = H_r$.

We shall now find explicit expressions for $U_+(t)$ in terms of the interaction V. If the expansions (3.3) and (3.12) converge, we get from (5.30) the following expressions for $U_+(t)$ and $U_-(t)$:

$$U_+(t)_* = \Psi_*(t) = \exp(E_{RL}\,t/i\hbar)\sum_{n=0}^{\infty}(\S\,V)^n \,\|\, = \sum_{n=0}^{\infty}(\S\,V(t))^n \,\| \tag{5.33}$$

or

$$U_+(t)_* = Q_*(t)\left(1+\frac{iK_*}{2}\right)^{-1} = Q_*(t)\sum_{n=0}^{\infty}\left(\frac{K_*}{2\,i}\right)^n, \tag{5.34}$$

$$U_-(t)_* = \Omega_*(t) = \sum_{n=0}^{\infty}(\flat\,V(t))^n \,\| = Q_*(t)\sum_{n=0}^{\infty}\left(\frac{iK_*}{2}\right)^n. \tag{5.35}$$

It should be remembered, however, that, according to the conclusion arrived at in Chapter III, the series (5.33)—(5.35) can converge for all of their matrix elements only if the system considered has no bound states. This at the same time will ensure the validity of the conditional equalities Eq. (5.30) from which Eqs. (5.33)—(5.35) were derived. In this same case we finally get for DYSON's S-matrix, by (5.33) with (1.27),

$$S_* = U_+(+\infty)_* = 1 + 2\sum_{n=1}^{\infty} \delta V (\S V)^{n-1} \|, \qquad (5.36)$$

which is identical with the expression (3.6) for HEISENBERG's S-matrix, in accordance with (5.31).

VI. Time-dependent perturbation treatment.

An alternative method of solution for Eqs. (5.4) and (5.8) is use of successive approximations. These equations are obviously equivalent with the integral equation

$$U(t, t_0) - 1 = \int_{t_0}^{t} \{V \exp(E_{RL} t_1/i\hbar)\} U(t_1, t_0)\, dt_1/i\hbar. \qquad (6.1)$$

Integrating by parts (hoping the best for contributions with $E_{RL} = 0$ in (6.1)), using (1.19), (5.4), and (5.8), we find (with $a \to 0$ in the definition of the slash),

$$\left.\begin{aligned} U(t, t_0) - 1 &= -\| V(t) ? U(t, t_0) + \| V(t_0) ? \\ &+ \int_{t_0}^{t} \{\| V ? \exp(E_{RL} t_1/i\hbar)\} V(t_1) U(t_1, t_0)\, dt_1/i\hbar. \end{aligned}\right\} \qquad (6.2)$$

Repeating this process n times, we get

$$\left.\begin{aligned} &\sum_{i=0}^{n} \| \{V(t) ?\}^i U(t, t_0) - \sum_{i=0}^{n} \| \{V(t_0) ?\}^i \\ &= \int_{t_0}^{t} \{\| (V ?)^n V \exp(E_{RL} t_1/i\hbar)\} U(t_1, t_0)\, dt_1/i\hbar. \end{aligned}\right\} \qquad (6.3)$$

The right—hand member contains the interaction energy V in the $(n+1)\,th$ power and must be assumed to go to zero for $n \to \infty$ if an expansion in powers of V is at all allowed.

Hence, we get

$$Y_*^{\dagger}(t)\, U(t, t_0) = Y_*^{\dagger}(t_0), \qquad (6.4)$$

where $Y_*(t)$ is obtained by (1.19) from Y_* as defined by (3.2), but with the meaning of the slash in (3.2) the conjugate by (1.8) of the meaning of the slash in (6.2)—(6.3).

Now, it was shown in Chapter III that the series Y_* and thus also $Y_*(t)$ converge only if the system has no bound states and, in that case, Y_* has a reciprocal and (6.4) can be solved uniquely with respect to $U(t, t_0)$. For instance, for the special choice that, in (6.3) $? = \flat$, so that $Y_* = \Psi_*$, we have, by (3.11),

$$\left.\begin{aligned} \Psi_*(t)\,\Psi_*(t)^\dagger = \Psi_*\,\Psi_*^\dagger \exp(E_{RL}\,t/i\hbar) = 1 \\ \Psi_*(t) = (\Psi_*(t)^\dagger)^{-1}. \end{aligned}\right\} \tag{6.5}$$

Thus, we get from (6.4) the solution

$$U(t, t_0) = \Psi_*(t)\,\Psi_*^\dagger(t_0), \tag{6.6}$$

which is in accordance with (5.19) if there are no bound states. In the limits $t_0 \to -\infty$ and $t \to +\infty$, (6.6) gives results which are identical with (5.33)—(5.36).

On the other hand, if there are bound states, the expansion Y_* cannot generally converge, and Y_* does not have a reciprocal. Therefore, the matrix elements of Eq. (6.4) do no longer define uniquely a propagation matrix $U(t, t_0)$, so that no information on the propagation of the bound states is obtained by a perturbation treatment.

VII. Interpretation of the time-dependent scattering matrix $\Psi(t)$ and of the matrix $\Psi(+\infty)$.

We return now to a problem left at the end of Chapter IV. It was stressed there that the Ψ-matrix gives a correct direct picture of a superposition of free-particle waves and outgoing scattered waves. This is true for the $\Psi(t)$ matrix as well. However, it was remarked that this was not true for the S-matrix which, contrary to the $\Psi(t)$-matrix, gives us a picture of as many incoming as outgoing scattered waves superimposed on the free-particle waves. This makes us wonder: If $\Psi(t)$ gives the correct picture for any large value of t, how is it possible that

$S = \Psi(+\infty)$ gives the wrong picture? We shall show that this is due partly to the fact that (5.26) is only a conditional equality and partly to an un-physical order of sequence of taking limits, which is automatically introduced by making use of the S-matrix in momentum space in interaction representation.

To see this, we have to recapitulate part of the well-known proof that a wave function of the form $\S F(t)\|$ asymptotically consists of outgoing waves only[9), 4)].

For interpretation of $\S F(t)\|$ in (2.23a) as a probability amplitude, we transform it back to xyz-space for one of the particles scattered. If $k = (\vec{k}, \cdots)$, where $\hbar\vec{k}$ is the momentum of the particle considered, we have in Schrödinger representation, omitting a normalization constant:

$$\left.\begin{aligned} T(x, \cdots, t) &= \int d^{(3)}k \, \exp(i\vec{k}\vec{x} + Et/i\hbar) \langle \vec{k} \cdots \cdots | \, \S F(t) \| \vec{k}_0 \cdots \rangle \\ &= \int_0^\infty k^2 \, dk \int_0^{2\pi} d\varphi \int_{-1}^{1} du \, e^{ikru} \, e^{Et/i\hbar} \, \frac{\langle \vec{k} \cdots \cdots | F | k_0 \cdots \cdots \rangle \, e^{[(E_0 \cdots) - (E \cdots)]\, t/i\hbar}}{(E_0 \cdots) - (E \cdots) + ia}. \end{aligned}\right\} \tag{7.1}$$

Here, $u = \cos\theta$, (we have taken $\vec{x}$ in the $+z$ direction) and E_0 and E are energies of the particle considered, while the dots stand for energies of other particles participating in the collision. Let E_1 be the value which E should take for conservation of energy, so that

$$(E_0 \cdots) - (E \cdots) = E_1 - E, \tag{7.2}$$

and let $\hbar k_1$ indicate the absolute value of the corresponding momentum. Further, putting

$$\left.\begin{aligned} \langle 0, 0, \pm k, \cdots \cdots | F | \vec{k}_0, \cdots \rangle &= F^{(\pm)}, \\ \langle 0, 0, \pm k_1, \cdots \cdots | F | \vec{k}_0, \cdots \rangle &= F_1^{(\pm)}, \end{aligned}\right\} \tag{7.3}$$

we get, asymptotically (for $r \to \infty$),[9), 4)]

$$T(0, 0, r, t) \approx \frac{2\pi \, e^{E_1 t/i\hbar}}{ir} \int_0^\infty k dk \, \frac{e^{ikr} F^{(+)} - e^{-ikr} F^{(-)}}{E_1 - E + ia}. \tag{7.4}$$

Because of the resonance for $a \to 0$ at $E = E_1$ we put

$$e^{\pm ikr} \approx e^{\pm ik_1 r} \cdot e^{\pm i\xi r/v_1\hbar}, \tag{7.5}$$

where

$$\xi \equiv E - E_1 \approx v_1 \hbar (k - k_1) \tag{7.6}$$

with

$$v = dE/\hbar dk. \tag{7.7}$$

We also use

$$EdE = c^2 \hbar^2 \, kdk, \tag{7.8}$$

and complete the path of integration in the complex ξ-plane to a contour via $\xi = \pm i\infty$ for the term with $F^{(\pm)}$. Only the contour for $F^{(+)}$ then encloses the pole at $\xi = +ia$, and we find for $a \to 0$

$$T(0, 0, r, t) \approx -(4\pi^2/rc^2\hbar^2) F_1^{(+)} E_1 \exp[ik_1(r - w_1 t)], \tag{7.9}$$

where we put

$$w_1 = c^2/v_1 = E_1/\hbar k_1. \tag{7.10}$$

Eq. (7.9) indeed represents an outgoing wave, however large t is.

The error made when one uses $S = \Psi(\infty)$for $\Psi(t)$, that is, using $\langle k \mid R \mid k_0 \rangle$ in (7.1) instead of $\langle k \mid T(t) \mid k_0 \rangle$, is in the first place in taking the limit $t \to \infty$ in the definition of R and S by

$$\langle k \mid R \mid k_0 \rangle = \lim_{t \to \infty} \langle k \mid T(t) \mid k_0 \rangle \tag{7.11}$$

(similar for S and Ψ), *before* this quantity is substituted into (7.1) and the integral over k performed. This amounts to not combining the factors $\exp(Et/i\hbar)$ and $\exp[(E_1 - E)\, t/i\hbar]$ in (7.1) to the harmless factor $\exp(E_1 t/i\hbar)$ of (7.4), but to writing

$$\left.\begin{aligned} T(0, 0, r, t) \approx \frac{2\pi}{ir} \int_0^\infty e^{Et/i\hbar} \int \frac{(\xi + E_1)\, d\xi}{\hbar^2 c^2 (ia - \xi)} \\ \times \left\{ F^{(+)} e^{ik_1 r} e^{i(v_1 t + r)\xi/v_1\hbar} - F^{(-)} e^{-ik_1 r} e^{i(v_1 t - r)\xi/v_1\hbar} \right\}, \end{aligned}\right\} \tag{7.12}$$

and then taking the limit $t \to \infty$ in the definition of the S-matrix in the factor on the second line only, while on the first line one puts $E \approx E_1$ on account of the resonance denominator. Thus, replacing $\Psi(\infty)$ by S in the transformation to xyz-space leads, from (7.12), wrongly to

$$R(0,0,r,t) \approx -\frac{4\pi^2 e^{E_1 t/i\hbar} E_1}{r\hbar^2 c^2} \lim_{\substack{r\to\infty \\ t\to\infty}} \Lambda, \tag{7.13}$$

where Λ is obtained by a contour via $\xi = +i\infty$ for the term with $F^{(+)}$, while for the term with $F^{(-)}$ the contour in the complex plane must be taken along $\xi = \pm i\infty$ as $v_1 t \gtrless r$:

$$\Lambda = F_1^{(+)} e^{ik_1 r} - F_1^{(-)} e^{-ik_1 r} \quad \text{if } v_1 t > r, \tag{7.14}$$

$$\Lambda = F_1^{(+)} e^{ik_1 r} \qquad \text{if } v_1 t < r. \tag{7.15}$$

We see that even with the error made we still would have found the correct result (7.9) if we had kept $v_1 t < r$, that is, if we study the asymptotic behaviour $r \to \infty > v_1 t$ for some possibly large, but anyhow finite time t. But, in using the S-matrix, the limit $t \to \infty$ has already been taken first inside the brackets on the second line of Eq. (7.12), *before* we take $r \to \infty$, yes, even before we transform at all from k-space to xyz-space. Therefore, the S-matrix (or rather its scattering part R) represents in xyz-space not (7.13) with (7.15), but (7.13) with (7.14), or

$$R(0,0,r,t) = -\frac{4\pi^2 E_1}{rc^2\hbar^2}\left\{F_1^{(+)} e^{ik_1(r-w_1 t)} - F_1^{(-)} e^{-ik_1(r+w_1 t)}\right\}, \tag{7.16}$$

which obviously contains incoming as well as outgoing waves.

Therefore, R does not depict the scattered wave. Only $T(t)$ should be used for this purpose.

In the sense of the conditional equalities (5.26), the collision process may be pictured as a steady transition from the state $\langle k \mid k_0 \rangle$ with definite values k_0 for the momenta at $t = -\infty$ to a state $\langle k \mid S \mid k_0 \rangle$ at $t = +\infty$, so that the probability $P(k)$ of finding the system with momenta $k \neq k_0$ after the collision is

$$P(k) = |\langle k|S|k_0\rangle|^2 = |\langle k|R|k_0\rangle|^2 = 4\pi^2 [\delta(E-E_0)]^2 |\langle k|F|k_0\rangle|^2,$$

where we have used (2.28) and (1.5). Since

$$[\delta(E-E_0)]^2 = h^{-1}\int_{-\infty}^{\infty} e^{i(E-E_0)t/\hbar}dt \cdot \delta(E-E_0) = \frac{\delta(E-E_0)}{h}\int_{-\infty}^{\infty} dt,$$

we have

$$P(k) = \frac{2\pi}{\hbar} T\delta(E-E_0)|\langle k|F|k_0\rangle|^2,$$

where T is the infinite time during which the collision has taken place. The probability density in k-space per unit time for a transition $k_0 \to k$ is thus[1)]

$$P_{k_0\to k} = \frac{2\pi}{\hbar}\delta(E-E_0)|\langle k|F|k_0\rangle|^2, \qquad (7.17)$$

where the δ-function takes care of energy conservation. Equation (7.17) is in accordance with the results quoted in the first part of Chapter IV.

As was shown in reference 5, the same result is obtained if the time derivative of the probability function

$$P(k, t) = |\langle k|\Psi(t)|k_0\rangle|^2$$

at time t is defined as*

$$\begin{aligned} P_{k_0\to k}(t) &= \frac{\partial}{\partial t}[\langle k|\Psi(t)|k_0\rangle^*\langle k|\Psi(t)|k_0\rangle] \\ &= \langle k_0|\Psi^\dagger(t)|k\rangle\frac{\partial}{\partial t}\langle k|\Psi(t)|k_0\rangle \\ &\quad + \left\{\frac{\partial}{\partial t}\langle k_0|\Psi^\dagger(t)|k\rangle\right\}\cdot\langle k|\Psi(t)|k_0\rangle \\ &= \frac{1}{i\hbar}\{\langle k_0|\Psi^\dagger(t)|k\rangle\langle k|V(t)\Psi(t)|k_0\rangle \\ &\quad - \langle k_0|\Psi^\dagger(t)V(t)|k\rangle\langle k|\Psi(t)|k_0\rangle\}, \end{aligned}$$

where we have used the Schrödinger equation (5.16) for the functions $\Psi(t)$ and $\Psi^\dagger(t)$. Using further (1.19), (2.23a)—(2.25a), we get

* The same idea appears in Eq (1.68) of reference 1.

$$P_{k_0\to k}(t) = \frac{1}{i\hbar}\{\langle k|k_0\rangle[\langle k_0|F|k_0\rangle - \langle k_0|F^\dagger|k_0\rangle]$$
$$+\langle k_0|T^\dagger|k\rangle\langle k|F|k_0\rangle - \langle k_0|F^\dagger|k\rangle\langle k|T|k_0\rangle\}$$
$$= \frac{1}{i\hbar}\{\langle k|k_0\rangle[\langle k_0|F^\dagger T|k_0\rangle - \langle k_0|T^\dagger F|k_0\rangle]$$
$$+\langle k_0|\,\|F^\dagger\flat\,|k\rangle\langle k|F|k_0\rangle - \langle k_0|F^\dagger|k\rangle\langle k|\S F\|\,|k_0\rangle\},$$

where we have used (2.33 a) and $\langle k|k_0\rangle = \delta(k-k_0)$. Finally, since by 1.9a

$$\flat(E_0-E) - \S(E_0-E) = +2\pi i\,\delta(E-E_0),$$

we get for the probability density in k-space per unit time of a transition $k_0 \to k$ at any time

$$\left.\begin{aligned} P_{k_0\to k} = \frac{2\pi}{\hbar}\Big\{&\delta(E-E_0)\,|\langle k|F|k_0\rangle|^2 \\ -\delta(k-k_0)&\int\delta(E_0-E')\,|\langle k'|F|k_0\rangle|^2\,dk'\Big\}. \end{aligned}\right\} \quad (7.18)$$

(7.18) is in accordance with "conservation of normalization":

$$\frac{\partial}{\partial t}\int\langle k_0|\Psi^\dagger|k\rangle\,dk\,\langle k|\Psi|k_0\rangle = \frac{\partial}{\partial t}\int P(k,t)\,dk = \int dk\,P_{k_0\to k} = 0$$

and, if $k \neq k_0$, (7.18) is identical with (7.17).

VIII. The methods of Källen and of Yang and Feldman[11].

In the preceding sections, the S-matrix has been defined in terms of the state functions either in Schrödinger representation or in interaction representation. Sometimes, in particular in field theories, it is more convenient to work in a Heisenberg representation and to derive the S-matrix directly from the field equations without an explicit use of the Hamiltonian and the Schrödinger equation.

Let ξ be any dynamical variable of the system in a Schrödinger representation, i. e. ξ is a time-independent matrix. In interaction representation, we then have the matrix

$$\left.\begin{aligned} \xi(t) &= \xi \exp(E_{RL}\, t/i\hbar), \\ \xi(t) &= \xi(t_0) \exp[E_{RL}(t-t_0)/i\hbar], \end{aligned}\right\} \tag{8.1}$$

where the interaction representation has been chosen identical with the Schrödinger representation at the time $t = 0$. Similarly, we may define a Heisenberg representation

$$\xi_H(t) = U^\dagger(t, 0)\, \xi(t)\, U(t, 0), \tag{8.2}$$

where $U(t, t_0)$ is the propagation matrix of Chapter V.

While the variables $\xi_H(t)$ satisfy the usual equations of motion with interaction, the $\xi(t)$ satisfy the corresponding equations of motion for a system with no interaction, i. e.

$$i\hbar\, d\xi(t)/dt = E_{RL}\, \xi(t). \tag{8.3}$$

For $t = 0$, we have, by our special choice of representations,

$$\xi_H(0) = \xi(0) = \xi. \tag{8.4}$$

We now introduce a new interaction representation[12] of the dynamical variables by matrices $\xi_{t_0}(t)$ depending on two time parameters t_0 and t. For a fixed t_0 they are defined as those solutions of the free particle equations of motion (8.3) which for $t = t_0$ coincide with the Heisenberg matrices $\xi_H(t_0)$, i. e.

$$\left.\begin{aligned} i\hbar\, d\xi_{t_0}(t)/dt &= E_{RL}\, \xi_{t_0}(t), \\ \xi_{t_0}(t_0) &= \xi_H(t_0). \end{aligned}\right\} \tag{8.5}$$

The solution of these equations may, by (8.1) and (8.2), be written as

$$\left.\begin{aligned} \xi_{t_0}(t) &= \xi_H(t_0) \exp[E_{RL}(t-t_0)/i\hbar] \\ &= \{U^\dagger(t_0, 0) \exp[E_{RL}(t-t_0)/i\hbar]\} \\ &\quad \times \xi(t) \{U(t_0, 0) \exp[E_{RL}(t-t_0)/i\hbar]\} \\ &= (\{U^\dagger(t_0, 0) \exp[-E_{RL}\, t_0/i\hbar]\} \\ &\quad \times \xi \{U(t_0, 0) \exp[-E_{RL}\, t_0/i\hbar]\}) \exp(E_{RL}\, t/i\hbar). \end{aligned}\right\} \tag{8.6}$$

From the expression (5.19) for the propagation matrix $U(t, t_0)$ we get at once

$$\left.\begin{aligned} U(t_0, 0)\exp(-E_{RL}\,t_0/i\hbar) &= \Psi\cdot\Psi^\dagger(-t_0)+\sum_r \psi_r\cdot\psi_r^\dagger(-t_0)\\ &= U(0,-t_0).\end{aligned}\right\} \tag{8.7}$$

This equation simply expresses the fact that the propagation matrix in the Schrödinger representation, i. e.

$$U_S(t, t_0) = e^{Et/i\hbar}\,U(t, t_0)\,e^{-Et_0/i\hbar}, \tag{8.8}$$

is a function of the difference $t - t_0$ only.

By (8.7) we get from (8.6)

$$\xi_{t_0}(t) = \left\{U^\dagger(0,-t_0)\,\xi\,U(0,-t_0)\right\}\exp(E_{RL}\,t/i\hbar). \tag{8.9}$$

The matrices $\xi_{t_0}(t)$ may also be interpreted as Heisenberg representatives of the dynamical variables of the system without interaction. Further, since each value of t_0 defines a space-like surface σ_0 in Minkowski space, viz. the surface of points with time coordinates equal to t_0, the variables $\xi_{t_0}(t)$ correspond to the field variables $\Psi(\sigma, x)$ in YANG and FELDMAN'S notation[11]. The connection between the variables $\xi_{t_0}(t)$ and $\xi_{t_1}(t)$ corresponding to two such surfaces σ_0 and σ_1, respectively, is by (8.9) given by the unitary transformation

$$\xi_{t_1}(t_0) = W^\dagger_{t_0 t_1}(t)\,\xi_{t_0}(t)\,W_{t_0 t_1}(t) \tag{8.10}$$

with

$$\left.\begin{aligned} W_{t_0 t_1}(t) &= \left\{U^\dagger(0,-t_0)\,U(0,-t_1)\right\}\exp(E_{RL}\,t/i\hbar)\\ &= U(-t_0,-t_1)\exp(E_{RL}\,t/i\hbar) = U(t-t_0, t-t_1),\end{aligned}\right\} \tag{8.11}$$

by (5.3b) and arguments similar to (5.2)—(5.3a) and (8.7)—(8.8).

We now define the in- and out-variables by

$$\left.\begin{aligned} \xi_{\text{in}}(t) &= \lim_{t_0\to-\infty}\xi_{t_0}(t), &\text{a)}\\ \xi_{\text{out}}(t) &= \lim_{t_1\to+\infty}\xi_{t_1}(t). &\text{b)}\end{aligned}\right\} \tag{8.12}$$

The connection between these variables is obtained from (8.10)—(8.11) by taking the limits $t_0 \to -\infty$, $t_1 \to +\infty$. From the definitions (5.25) of the $U_+(t)$ matrix and Dyson's definition (5.31) of the S-matrix, we get

$$\left.\begin{aligned} \lim_{\substack{t_0 \to -\infty \\ t_1 \to +\infty}} U(-t_0, -t_1) = \lim_{\substack{t_0 \to -\infty \\ t_1 \to +\infty}} U(t_1, t_0) = \lim_{t_1 \to +\infty} U_+(t_1) = S. \end{aligned}\right\} \quad (8.13)$$

Hence, by (8.12), (8.10), and (8.11)

$$\xi_{\text{out}}(t) = S^\dagger \xi_{\text{in}}(t) S, \quad (8.14)$$

i. e. the in- and out-variables are connected by a unitary transformation with the S-matrix as transformation matrix. Since the relation between in- and out-variables may be obtained by solving the equations of motion for $\xi_H(t)$, (8.14) represents a way of determining the S-matrix without the use of Hamiltonian or Schrödinger equation. These methods of KÄLLÉN and of YANG and FELDMAN have proved to be useful in field theory[12], and may be applied also in cases where the system is not a Hamiltonian system. For Hamiltonian systems, it is easy to find the connection between the in- and out-variables and the matrices Ω and Ψ. By (5.25) and (5.30) we get

$$\left.\begin{aligned} \lim_{t_0 \to -\infty} U(0, -t_0) = U(0, +\infty) = {''}U_-(0) = \Omega'', \\ \lim_{t_1 \to +\infty} U(0, -t_1) = U(0, -\infty) = {''}U_+(0) = \Psi''. \end{aligned}\right\} \quad (8.15)$$

Hence, by (8.12) and (8.9),

$$\left.\begin{aligned} {''}\xi_{\text{in}}(t) = \left\{\Omega^\dagger \xi \Omega\right\} \exp\left(E_{RL}\, t/i\hbar\right) = \Omega^\dagger(t)\, \xi(t)\, \Omega(t)'', \\ {''}\xi_{\text{out}}(t) = \left\{\Psi^\dagger \xi \Psi\right\} \exp\left(E_{RL}\, t/i\hbar\right) = \Psi^\dagger(t)\, \xi(t)\, \Psi(t)'', \end{aligned}\right\} \quad (8.16)$$

which is in accordance with (8.14) on account of (2.48).

IX. Switching on and off the interaction.

Although the results thus far obtained are satisfactory, the treatment of the limits $t \to \pm\infty$ remains awkward. Trying to define the U_+-matrix as limit for $t_0 \to -\infty$ of the matrix $U(t, t_0)$ we were trying in fact to solve the Schrödinger equation for $U_+(t)$ with initial condition $U_+(t_0) = 1$ without stating the exact value of the time t_0. As, on account of the Schrödinger equation, $U_+(t)$ does not stay constant, this problem does not really make sense. Our procedure of then looking for a solution for $U_+(t)$ which is "unity on the average" for $t \to -\infty$ is only a makeshift, and leads to the complication that items that do not vanish at all (such as $\psi_r(t)$) yet may happen to vanish on the average for $t \to -\infty$.

We shall therefore try to solve this problem now by assuming that $V \to 0$ for $t \to \pm\infty$, so that we may really have $U_+(t) \to 1$ for $t \to -\infty$ and also a well defined limit of $U_+(t)$ for $t \to +\infty$. For this purpose, we replace V in the original Schrödinger equation (2.3) by

$$V \exp(-a|t|/\hbar) \tag{9.1}$$

with extremely small, but finite positive a.

Inserting (9.1) in the definition (1.19) of the matrix $V(t)$ occurring in (2.6), and therefore also appearing in Eq. (5.4), we have for the non-closed system in interaction representation a potential

$$V(a; t) = V \exp[(E_{RL}\, t - ia|t|)/i\hbar]. \tag{9.2}$$

Thence, we have to solve the equations

$$i\hbar\, \partial U_+(a; t)/\partial t = \{V \exp(E_{1,RL}\, t/i\hbar)\}\, U_+(a; t) \text{ for } t < 0 \tag{9.3}$$

and

$$i\hbar\, \partial U_+(a; t)/\partial t = \{V \exp(E_{-1,RL}\, t/i\hbar)\}\, U_+(a; t) \text{ for } t > 0 \tag{9.4}$$

with the initial condition

$$U_+(a; -\infty) = 1. \tag{9.5}$$

Here we have put

$$E_{n,RL} = E_{RL} + nia, \tag{9.6}$$

and we shall also introduce a generalized scat $\S_n$ for a division by $(E_{\|} - E_{\S} + nia)$. Thus, $\S_1$ is equal to $\S$, with the difference that now a is not necessarily going to zero. Similarly, we introduce a generalized flat $\flat_n$ for a division by $(E_{\|} - E\flat - nia)$.

By $\Phi(a;t)$ we shall denote the solution of the differential equation (9.3) which has the limit 1 for $t \to -\infty$:

$$\lim_{t\to-\infty} \Phi(a;t) = 1. \tag{9.7}$$

Similarly, $X(a;t)$ shall denote the solution of (9.4) satisfying the condition

$$\lim_{t\to+\infty} X(a;t) = 1. \tag{9.8}$$

Assuming that the limits in (9.7)—(9.8) give real (and not only conditional) equality of Φ at $-\infty$ and of X at $+\infty$ to unity, we conclude that

$$\left.\begin{aligned} \Phi^{\dagger}(a;-\infty)\,\Phi(a;-\infty) = \Phi(a;-\infty)\,\Phi^{\dagger}(a;-\infty) = 1, \\ X^{\dagger}(a;+\infty)\,X(a;+\infty) = X(a;+\infty)\,X^{\dagger}(a;+\infty) = 1. \end{aligned}\right\} \tag{9.9}$$

Now, consider the matrices $\langle k|\Phi(a;t)|k_0\rangle$ and $\langle k|X(a;t)|k_0\rangle$ as two sets of functions of k, labeled by k_0. At $t = -\infty$, the first set of functions is, by (9.9), a complete orthonormal set and, on account of the conservation of orthonormality and completeness of a set of solutions of the Schrödinger equation, which was shown in Eqs. (5.10)—(5.11) to hold also for non-closed systems, we have for any finite time t

$$\Phi^{\dagger}(a;t)\,\Phi(a;t) = \Phi(a;t)\,\Phi^{\dagger}(a;t) = 1. \tag{9.10}$$

By the same argument, we get from (9.9)

$$X^{\dagger}(a;t)\,X(a;t) = X(a;t)\,X^{\dagger}(a;t) = 1. \tag{9.11}$$

If the series converge, we get an explicit expression for $\Phi(a;t)$ in terms of the potential V by

$$\left.\begin{aligned}\Phi_*(a;t) &= 1+\sum_{n=1}^{\infty}\left\{\prod_{i=0}^{n-1}(\S_{n-i}V)\,\|\right\}\exp\,(E_{n,RL}\,t/i\hbar)\\ &= 1+\S_1 V\|\exp\,(E_{1,RL}\,t/i\hbar)\\ &+\S_2 V\S_1 V\|\exp\,(E_{2,RL}\,t/i\hbar)+\cdots\\ &+\S_n V\S_{n-1}V\cdots\S_2 V\S_1 V\|\exp\,(E_{n,RL}\,t/i\hbar)+\cdots.\end{aligned}\right\}\quad(9.12)$$

Indeed, in $i\hbar\,\partial\Phi_*(a;t)/\partial t$ all first factors $\S_n$ are canceled, and by

$$VA\exp\,(E_{n,RL}t/i\hbar)\}=\{V\exp\,(E_{1,RL}\,t/i\hbar)\}\{A\exp\,(E_{n-1,RL}t/i\hbar)\}\quad(9.13)$$

we may factorize out $\{V\exp(E_{1,RL}\,t/i\hbar)\}$ from the resulting expression and just obtain $\{V\exp(E_{1,RL}\,t/i\hbar)\}\Phi_*(a;t)$.

Since $a>0$, all terms but the first in (9.12) vanish for $t\to-\infty$, which takes care of the initial condition

$$\Phi_*(a;-\infty)=1.$$

In the same way, one sees that the series

$$\left.\begin{aligned}\chi_*(a;t) &= 1+\sum_{n=1}^{\infty}\left(\prod_{i=0}^{n-1}\flat_{n-i}V\right)\|\exp\,(E_{-n,RL}\,t/i\hbar)\\ &= 1+\flat_1 V\|\exp\,(E_{-1,RL}\,t/i\hbar)\\ &+\flat_2 V\flat_1 V\|\exp\,(E_{-2,RL}\,t/i\hbar)+\cdots\cdots\\ &+\flat_n V\flat_{n-1}V\cdots\flat_2 V\flat_1 V\|\exp\,(E_{-n,RL}\,t/i\hbar)+\cdots\end{aligned}\right\}\quad(9.14)$$

is a solution of (9.4) satisfying the condition $X_*(a;+\infty)=1$, provided, of course, that the series is convergent.

Since $U_+(t)$ is that solution of the Schrödinger equation with the potential (9.2) which is continuous at $t=0$ and satisfies the initial condition (9.5), we have

$$U_+(a;t) = \left\{ \begin{array}{ll} \Phi(a;t) & \text{for } t<0, \\ X(a;t)\,X(a)^\dagger\,\Phi(a) & \text{for } t>0, \end{array} \right\} \quad (9.15)$$

where

$$\Phi(a) = \Phi(a;t\,0),\ X(a) = X(a;0) \quad (9.16)$$

denote the values of $\Phi(a;t)$ and $X(a;t)$ for $t=0$. The expression (9.15) for $U_+(a;t)$ is seen to be continuous at $t=0$ and unitary for all t, on account of (9.10), (9.11):

$$U_+^\dagger(a;t)\,U_+(a;t) = U_+(a;t)\,U_+^\dagger(a;t) = 1. \quad (9.17)$$

For an arbitrary state $\langle k \mid \psi(a;t)$ of the non-closed system with $a \neq 0$, we now obviously have

$$\psi(a;t) = U_+(a;t)\,\psi(a;-\infty), \quad (9.18)$$

where $\psi(a;-\infty)$ is the value of $\psi(a;t)$ for $t=-\infty$. Indeed, (9.18) is a solution of the Schrödinger equation of the non-closed system and (9.5) takes care of the initial condition.

From (9.17) and (9.18) we get

$$\psi(a;-\infty) = U_+^\dagger(a;t)\,\psi(a;t). \quad (9.19)$$

Hence,

$$\psi(a;t) = U_+(a;t)\,U_+^\dagger(a;t_0)\,\psi(a;t_0) \equiv U(a;t,t_0)\,\psi(a;t_0), \quad (9.20)$$

i. e.

$$U(a;t,t_0) = U_+(a;t)\,U_+^\dagger(a;t_0) \quad (9.21a)$$

and

$$U_+(a;t) = \lim_{t_0 \to -\infty} U(a;t,t_0) \quad (9.21b)$$

on account of (9.5).

If we now define a matrix $S(a)$ as the limit of $U_+(a;t)$ for $t \to +\infty$, we get, by (9.15) and (9.8),

$$S(a) = \lim_{t\to+\infty} U_+(a;t) = X^\dagger(a)\,\Phi(a) = \lim_{\substack{t_0\to-\infty \\ t\to+\infty}} U(a;t,t_0), \quad (9.22)$$

which is unitary on account of (9.10)—(9.11). Hence, $S(a)$ is the Dyson S-matrix for the non-closed system where the interaction is switched on and off. In contrast to the Heisenberg S-matrix, the matrix $S(a)$, according to (9.22), with (9.16), (9.12), (9.14), (1.7), does not contain a factor $\delta(E_{RL})$. This is connected with the fact that the energy is not conserved in the system with $a > 0$. By (9.18), $S(a)$ is the matrix which connects any state vector at $t = -\infty$ with the state vector at $t = +\infty$ by

$$\psi(a; +\infty) = S(a)\,\psi(a; -\infty). \tag{9.23}$$

In all these expressions we shall now go to the limit of $a \to 0$, but we shall first assume that the series (9.12) and (9.14) for $t = 0$, i. e. the series $\Phi_*(a) \equiv \Phi_*(a; 0)$ and $X_*(a) \equiv X_*(a; 0)$, are uniformly convergent for all a including the value $a = 0$, so that we can take the limit $a \to 0$ term by term in the expansions. Since $\S_n \to \S$ and $\flat_n \to \flat$ for $a \to 0$, we then get

$$\left.\begin{aligned} \Phi_*(0) &= \sum_{n=0}^{\infty} (\S\, V)^n \,\| = \Psi_* \\ X_*(0) &= \sum_{n=0}^{\infty} (\flat\, V)^n \,\| = \Omega_* \end{aligned}\right\} \tag{9.24}$$

on account of (3.3a), (3.3b). As was seen in Chapter III, these series can converge only if the system considered has no bound states. The assumption made above about the uniform convergence of $\Phi(a)$ and $X(a)$ can therefore only be justified when no bound states exist. In this case, however, we get from (9.12) and (9.14), by $E_{\pm n, RL} \to E_{RL}$ for $a \to 0$,

$$\left.\begin{aligned} \Phi_*(0; t) &= \sum_{n=0}^{\infty} (\S\, V(t))^n \,\| = \Psi_*(t) \text{ for } t < 0, \\ X_*(0; t) &= \sum_{n=0}^{\infty} (\flat\, V(t))^n \,\| = \Omega_*(t) \text{ for } t > 0. \end{aligned}\right\} \tag{9.25}$$

Thus, from (9.15), (9.24), (9.25), (2.47a), and using the relation

$$\Psi(t) = \Omega(t)\, S \tag{9.26}$$

following from (2.48), we find that, in this case,

$$U_+(0;t)_* = \lim_{a\to 0} U_+(a;t)_* = \Psi_*(t) \tag{9.27}$$

for all values of t. This equation is in agreement with the unitarity of U_+, as the system considered had no bound states. For such systems, Eq. (9.27) is a justification of the expectation expressed at the beginning of Chapter V, since the state $U_+(0;t)$, which at $t=-\infty$ represents an initial free particle state k_0, for finite times will have developed into the stationary state $\langle k \mid \Psi(t) \mid k_0 \rangle$.

Further, we get for such systems, from (9. 21 a), (9.27), and (5.19)—(5.21),

$$\lim_{a\to 0} U_*(a;t,t_0) = \Psi_*(t)\,\Psi_*^{\dagger}(t_0) = S_*(t,t_0) = U_*(t,t_0), \tag{9.28}$$

For these systems, the limit of $S(a)$ defined by (9.22) is also the S-matrix of HEISENBERG, since by (9.22), (9.24), and (2.47 a)

$$\lim_{a\to 0} S_*(a) = X^{\dagger}{}_*(0)\,\Phi_*(0) = \Omega^{\dagger}{}_*\,\Psi_* = \Omega^{\dagger}{}_*\,\Omega_*\,S_* = S_*. \tag{9.29}$$

Thus, in the case considered, the method of an infinitely slowly switching on and switching off the interaction leads in every respect to the same results as the method used in Chapter V for a strictly closed system with the conventions (1.23)—(1.32) for taking the limits $t\to\pm\infty$. The two methods differ only by the sequence in which the limits $a\to 0$ and $t\to\pm\infty$ are taken and, at least as far as our series expansions are sufficiently convergent, it does not matter which limit is taken first.

It is generally believed that this result holds also in cases, where the series expansions do not converge, for instance, also for systems with bound states. In particular, it is believed that an equation like (9.27) must always be valid on account of the "adiabatic theorem" of quantum mechanics[13] which states that a stationary state of a closed system by an adiabatic, i. e. infinitely slow, change of the potential goes over into the corresponding stationary state of the closed system with the new potential. The proof of the adiabatic theorem given by BORN and FOCK is, how-

ever, based on special assumptions about the potential and the type of energy spectrum, and to our knowledge no general proof of this theorem has ever been given.

X. Conclusion.

The purpose of a theory of collision processes is the calculation of differential and total scattering cross sections. The technique of obtaining these quantities from the matrices discussed in the foregoing was discussed in more detail in reference 4. From the discussions of Chapter VII of the present paper, however, it is clear that scattering is described most directly by the matrix Ψ defined by the integral equation (2.27 a). In fact, in Eq. (7.18) we obtained the density in momentum space of the transition probability per second directly in terms of the "effective potential" F, which by Eq. (2.25 a) is the product of the interaction operator V into the matrix Ψ. In the integration over final states in a given region in k-space, conservation of energy is then ensured by the delta function appearing in Eq. (7.18).

As shown in Chapter VII, the Heisenberg S-matrix in xyz-space for $t \to \infty$ gives an incorrect picture of the scattering phenomenon, since, due to the wrong order of sequence of limits, it describes incoming as well as outgoing spherical waves in such interpretation. When interpreted as a probability amplitude in momentum space, as in the reasoning preceding Eq. (7.17), it is seen to determine only an infinite transition probability during an infinite time. Although, by an artifice, one succeeds in obtaining Eq. (7.17) from such attempt at a direct interpretation of the S-matrix, a more satisfactory treatment was given by Eq. (4.1), in which the right-hand member amounts to factorizing a delta function $\delta(E_{RL})$ out of the matrix $R = S - 1$ by writing

$$S - 1 = R = \delta(E_{RL})\,\overline{R}; \quad \overline{R} = \int R\, dE_{RL} = \int (S-1)\, dE_{RL}. \quad (10.1)$$

A comparison of (10.1) with Eq. (2.28), in which the delt had the meaning defined in (1.5), shows that

$$(i/\pi)\ \delta\overline{R}\,\| = R = 2\ \delta F\,\|\,; \qquad \overline{R} = (2\pi/i)\ F\big|_{E_{RL}=0}. \quad (10.2)$$

Equation (10.2) relates $\overline{R}$ to F "on the energy shell", that is, to the matrix elements $\langle L|F|R\rangle$ with $E_{RL}=0$ only. Outside the energy shell, $\overline{R}$ is not really defined by (10.1). Because of the delta functions in Eq. (7.18), F in that equation may now be replaced by $(i/2\pi)\,\overline{R}$, so that

$$\left.\begin{aligned} P_{k_0\to k} = h^{-1}\Big\{ &\delta(E-E_0)\,|\langle k|\,\overline{R}\,|k_0\rangle|^2 \\ -\,\delta(k-k_0)\int &\delta(E_0-E')\,|\langle k'|\,\overline{R}\,|k_0\rangle|^2\,dk'\Big\}. \end{aligned}\right\} \tag{10.3}$$

Thus, by (10.1)—(10.3), cross sections for scattering in a finite time interval may be obtained from the S-matrix without need of the consideration of infinite probabilities preceding Eq. (7.17).

This reasoning is, of course, based primarily on combining the definition (2.28) of the Heisenberg S-matrix with the original definition of the Ψ-matrix as a set of probability amplitudes for given scattering states characterized by the momentum k_0 of the incident particles. If any different definition of the S-matrix is used, its equivalence is first to be proved; and, since the matrix Ψ is used, it has to be investigated to what extent every possible state of a given system of interacting particles can be described by it. This was the aim of the preceding chapters. The main results obtained, old and new ones, are the following.

While the S-matrix is always unitary [Eq. (2.45)], the Ψ-matrix in general is not so [Eq. (2.40)], while the scattering matrix Q symmetric in incoming and outgoing waves, which was defined by the integral equation (2.27c), is never unitary [Eq. (2.34c)]. The latter matrix is related to the Hermitian reaction matrix K by Eq. (2.29) with (2.25c) or with (2.23c)—(2.24c). The reaction matrix K, on the other hand, is related to the S-matrix by Eq.(2.44), and can be used for calculating phase shifts by means of (2.49)—(2.51) (cf. reference 1). Further relations between the matrices Ψ, Q, S, and K are found in Appendix D.

The propagation matrix $U(t, t_0)$, defined by Eq. (5.2) and expressed in terms of Ψ by (5.19), has been used by DYSON for defining an S-matrix called $U_+(\infty)$. This Dyson S-matrix relates the "in"- and "out"-variables of KÄLLÉN, YANG, and FELDMAN by Eq. (8.14). These variables may be interpreted as simply two

different interaction representations of the same quantities; the "in" representation coinciding (as far as this is possible) with the Heisenberg representation in the infinite past, and the "out" representation in the infinite future. They also are the Heisenberg representations of those solutions of the "homogeneous" field equations without interaction which describe incoming or outgoing particles. (Cf. references 11 and 12).

The definitions of $U_+(t)$ [Eq. (5.25)], of the Dyson S-matrix $U_+(\infty)$, and of the in and out variables are not quite satisfactory, unless one assumes that the interaction has been switched on since $t = -\infty$, and will be switched off before $t = +\infty$. In Chapter IX, we defined scattering matrices for finite switching-on and-off velocities. Now, $U_+(a; t)$ is given by Eq. (9.15), and $S(a)$ of Eq. (9.22) is the new Dyson S-matrix. The limits $t \to \pm\infty$ this time have been taken first. Little can be said in general about the properties of this matrix $S(a)$, which for finite a does not even ensure conservation of energy.

All these results are quite general; for actual calculations, however, some special assumptions have to be made. The least of these assumptions is the one discussed on pages 20-21 and in Appendix D, that the scattering matrices Ψ, Ω, and Q all three span the same subspace in Hilbert space. This enables us to derive the relations (2.48), (5.24), and (9.26) between the various scattering matrices.

A treatment of the limits $t \to \pm\infty$ without taking refuge to switching on and off the interaction leads to the "conditional equalities" (5.26)—(5.32) and (8.15)—(8.16). These formulas are usually supposed to prove the general equality of the Dyson S-matrix to the Heisenberg S-matrix. However, this treatment makes sense only in so far as bound states can be ignored, as seen from Eq. (5.28), or by comparing (5.32) with (2.40). In the more satisfactory treatment of Chapter IX, progress in this proof could be made only by assuming convergence of the series expansions of perturbation theory. More specifically, we assumed uniform convergence of the expansions (9.12)—(9.14) for all switching-on-and-off velocities of the field including the case where this velocity tends to zero. Then, the "improved" version of the Dyson S-matrix given by (9.22) was shown in Eq. (9.29) to yield the Heisenberg S-matrix in the final limit $a \to 0$.

However, in Chapter III it has been shown in complete generality that the expansions of perturbation theory for Ψ used in Chapter IX cannot possibly generally converge, if any bound states for the system are possible at all. (Any state, in which not all final particles go off to infinity, is here considered a "bound state"). This proof is based on the disagreement between Eqs. (3.11) and (2.40). For the exceptional systems for which no such bound states are possible, however, we have expressed all scattering matrices and related quantities explicitly in the form of expansions. [See Eqs. (3.3)—(3.6), (5.33)—(5.36), (9.12), (9.14)]. In the even more exceptional case that these expansions really converge, these expansions satisfy all equations derived for the quantities which they represent.

Concluding we may say that we have not been able to give a proof of the equality of the Dyson S-matrix and the Heisenberg S-matrix general enough to be valid also for systems with bound states. (We purposely omitted some arguments possible on the basis of an "adiabatic theorem" which we could not rigorously prove for the systems considered). It should, however, be remembered that cross sections are determined by Eqs. (7.18) or (10.3) without any discussion of what is going on at $t \to \pm\infty$. In principle, F in Eq. (7.18) can be found by direct solution of the integral equation (2.27a) and subsequent use of Eq. (2.25a); or $\overline{R}$ in Eq. (10.3) can be found by first solving for Q from Eq. (2.27c) and then finding W, K, R, and $\overline{R}$ by means of Eqs. (2.25c), (2.29), (2.43), and (10.1), respectively. The integral equations (2.27) retain their validity for systems with bound states.

Not discussed in this review of scattering theory are such problems as (1) the use of exact wave functions instead of the nth-order Born approximation involved in our representation of the scattering matrices in k-space and in our treatment of all but kinetic energy as the perturbation causing the scattering phenomenon; (2) explicit solution of collision problems for systems allowing bound states; (3) use of the method of analytic continuation of the S-matrix in the complex energy plane for obtaining additional information on systems of interacting particles; or (4) solution of scattering problems by variational methods.

Appendices.

A. We shall here prove the important relation (1.17):

$$D_{LR}\,D_{LM}+D_{RM}\,D_{LM}+D_{RM}\,D_{RL}=\pi^2\,\delta\,(E_{LM})\,\delta\,(E_{MR}) \tag{A.1}$$

with D_{RL} given by (1.5). This equation will be proved if, for an arbitrary function $f(E_L, E_M)$, the relation

$$\left.\begin{aligned} X\equiv\lim_{a\to 0}\iint dE_L\,dE_M\,f(E_L, E_M)\\ \times\left\{D_{LR}\,D_{LM}+D_{RM}\,D_{LM}+D_{RM}\,D_{RL}\right\}=\pi^2\,f(E_R, E_R)\end{aligned}\right\} \tag{A.2}$$

can be shown. To this purpose, we introduce new variables of integration $x = E_{LR}/a$ and $y = E_{MR}/a$, so $E_{LM} = a\,(x-y)$.

Let $f(E_L, E_M)\equiv g\,(E_{LR}, E_{MR})$; then,

$$\left.\begin{aligned} X&=\lim_{a\to 0}\int\!\!\int_{-\infty}^{\infty} dx\,dy\,g\,(ax, ay)\left\{\frac{x\,(x-y)}{(x^2+1)\,[(x-y)^2+1]}\right.\\ &\left.+\frac{y\,(y-x)}{(y^2+1)\,[(y-x)^2+1]}+\frac{xy}{(x^2+1)\,(y^2+1)}\right\}\\ &=\lim_{a\to 0}\int\!\!\int_{-\infty}^{\infty} dx\,dy\,g\,(ax, ay)\,\frac{x^2-xy+y^2}{(x+i)(x-i)(y^2+1)(x-y+i)(x-y-i)}.\end{aligned}\right\} \tag{A.3}$$

As the integrand vanishes at infinity as x^{-2}, we may close the contour in the complex x-plane; for instance, in positive direction through $+\,i\,\infty$ around the poles i and $y+i$. Thus, (A.3) yields

$$
\left.\begin{aligned}
X &= \lim_{a\to 0} 2\pi i \int_{-\infty}^{\infty} dy \\
&\times \left[\frac{[-1-iy+y^2]\, g\,(ia, ay)}{2i(y^2+1)(2i-y)(-y)} + \frac{[-1+iy+y^2]\, g\,(ay+ia, ay)}{(2i+y)\, y\,(y^2+1)\, 2i} \right] \\
&= \pi^2 \lim_{a\to 0} [\, g\,(ia, 2ia) + g\,(2ia, ia) - g\,(ia, ia)] \\
&= \pi^2\, g\,(0, 0) = \pi^2 f(E_R, E_R),
\end{aligned}\right\} \text{(A.4}
$$

which completes the proof of (A.2) and (A.1) or (1.17).

B. Next, we shall show by direct multiplication of the series (3.7) that $\Psi_*^\dagger \Psi_* = 1$. By (3.7) we have

$$
\Psi_*^\dagger \Psi_* = \sum_{n=0}^{\infty} A_n = \sum_{n=0}^{\infty} \left(\sum_{l=0}^{n} \| (V\flat)^l \cdot (\S\, V)^{n-l} \| \right) \qquad \text{(B.1)}
$$

with

$$
A_0 = 1, \; A_1 = \S\, V\| + \| V\flat = 0 \qquad \text{(B.2)}
$$

and, for $n \geq 2$,

$$
\left.\begin{aligned}
\langle L|A_n|R\rangle &= \int \langle L|\, V\,|k_1\rangle\, dk_1 \langle k_1|\, V\,|k_2\rangle\, dk_2 \cdots dk_{n-1} \langle k_{n-1}|\, V\,|R\rangle S(n), \\
S(n) &= \sum_{l=0}^{n} B_l(n), \\
B_l(n) &= \prod_{i=1}^{l} (E_L - E_i - ia)^{-1} \cdot \prod_{j=l}^{n-1} (E_R - E_j + ia)^{-1}.
\end{aligned}\right\} \text{(B.3}
$$

Here, $\prod_{i=1}^{0} (E_L - E_i - ia)^{-1}$ and $\prod_{j=n}^{n-1} (E_R - E_j + ia)^{-1}$ both mean 1, further E_i means E_R for $i = l = n$ and E_j means E_L for $j = l = 0$.

From these definitions we get the following connection between the expressions $B_l(n+1)$ and $B_l(n)$:

$$\left.\begin{aligned} B_l(n+1) &= B_l(n)\,(E_R - E_n + i\alpha)^{-1} \text{ for } 0 \leq l < n \\ B_n(n+1) &= B_n(n)\,\frac{E_L - E_R - i\alpha}{(E_L - E_n - i\alpha)\,(E_R - E_n + i\alpha)} \\ B_{n+1}(n+1) &= B_n(n)\,(E_L - E_n - i\alpha)^{-1}. \end{aligned}\right\} \quad \text{(B.4)}$$

Hence,

$$\left.\begin{aligned} S(n+1) &= \sum_{l=0}^{n-1} B_l(n+1) + B_n(n+1) + B_{n+1}(n+1) \\ &= \sum_{l=0}^{n} B_l(n)\cdot(E_R - E_n + i\alpha)^{-1} \\ &\quad + B_n(n)\left[-(E_R - E_n + i\alpha)^{-1} + \frac{E_L - E_R - i\alpha}{(E_L - E_n - i\alpha)\,(E_R - E_n + i\alpha)}\right. \\ &\qquad\qquad \left. + (E_L - E_n - i\alpha)^{-1}\right]. \end{aligned}\right\} \quad \text{(B.5)}$$

Since the last term in this expression is equal to

$$B_n(n)\,\frac{i\alpha}{(E_L - E_n - i\alpha)\,(E_R - E_n + i\alpha)},$$

it goes to zero as $\alpha \to 0$, and we get from (B.5) the formula

$$S(n+1) = S(n)\cdot(E_R - E_n + i\alpha)^{-1}. \quad \text{(B.6)}$$

Now, for $n = 2$, we have

$$\left.\begin{aligned} S(2) &= (E_R - E_L + i\alpha)^{-1}(E_R - E_1 + i\alpha)^{-1} \\ &\quad + (E_L - E_1 - i\alpha)^{-1}(E_R - E_1 + i\alpha)^{-1} \\ &\quad + (E_L - E_1 - i\alpha)^{-1}(E_L - E_R - i\alpha)^{-1} \\ &= \frac{i\alpha}{(E_L - E_1 - i\alpha)\,(E_L - E_R - i\alpha)\,(E_R - E_1 + i\alpha)} = 0 \text{ for } \alpha \to 0. \end{aligned}\right\} \quad \text{(B.7)}$$

Hence,

$$S(n) = 0 \text{ for } n \geq 2, \quad \text{(B.8)}$$

i. e., by (B.2), (B.3) and (B.1),

$$\left.\begin{aligned} A_n &= 0 \text{ for } n \geq 1, \\ \Psi_*^\dagger \Psi_* &= 1. \end{aligned}\right\} \tag{B.9}$$

Besides (B.9) we have, however, also

$$\Psi_* \Psi_*^\dagger = 1. \tag{B.10}$$

To complete the proof of this equation, we have, according to the considerations of Chapter III, Eqs. (3.7)—(3.11), only to show that the quantities

$$\left. B(n) = \sum_{l=0}^{n} \prod_{i=0}^{l-1} (E_l - E_i + ia)^{-1} \prod_{j=l+1}^{n} (E_l - E_j - ia)^{-1} \text{ for } n \geq 2 \right\} \tag{B.11}$$

are either identically zero or at least contain a factor a and, hence, go to zero for $a \to 0$. In (B.11), $\prod_{i=0}^{-1} (E_0 - E_i + ia)^{-1}$ and $\prod_{j=n+1}^{n} (E_n - E_j - ia)^{-1}$ both mean 1. A common denominator D of the fractions in the sum (B.11) is

$$D = \prod_{0 \leq i < j \leq n} (E_i - E_j - ia), \tag{B.12}$$

where the product is extended over all pairs of indices $i < j$ among the numbers 0, 1, 2 ... n. Hence,

$$B(n) = \frac{N(a; E_0, E_1, \cdots E_n)}{D}, \tag{B.13}$$

where the numerator N is given by

$$\left.\begin{aligned} N(a; E_0 \cdots E_n) &= \sum_{l=0}^{n} \frac{\prod_{0 \le i < j \le n} (E_i - E_j - ia)}{(-1)^l \prod_{0 \le i < l} (E_i - E_l - ia) \cdot \prod_{l < j \le n} (E_l - E_j - ia)} \\ &= \sum_{l=0}^{n} (-1)^l \prod_{0 \le i < j \le n}{}' (E_i - E_j - ia). \end{aligned}\right\} \quad \text{(B.14)}$$

Here, the prime on $\prod$ means that, in the product over all index pairs $i < j$, the factors with $i = l$ and $j = l$ should be left out. $N(a; E_0 \cdots E_n)$ is an algebraic function of the variables $(a; E_0, E_1, \cdots E_n)$ which has no singularities for any value of these variables. Further, we see that

$$N(a; E_0, \cdots E_n) = N(E_0 \cdots E_n) + N_1, \qquad \text{(B.15)}$$

where

$$N(E_0, \cdots E_n) = \sum_{l=0}^{n} (-1)^l \prod_{0 \le i < j \le n}{}' (E_i - E_j) = N(0; E_0 \cdots E_n) \quad \text{(B.16)}$$

is the function obtained by putting $a = 0$ in (B.14), while N_1 is a function which contains at least one factor a.

Thus, our statement will be proved if we can show that $N(E_0, \cdots E_n)$ is identically zero for all values of the independent variables $(E_0, E_1 \cdots E_n)$. Let us first assume that all variables $E_0, \cdots E_n$ are different and different from zero; then we can take out an l-independent factor $\prod_{0 \le i < j \le n} (E_i - E_j)$ and we get

$$N = \prod_{0 \le i < j \le n} (E_i - E_j) \cdot C(n), \qquad \text{(B.17)}$$

where

$$\left.\begin{aligned} C(n) &= \sum_{l=0}^{n} (-1)^l \frac{1}{\prod_{0 \le i < l} (E_i - E_l) \cdot \prod_{l < j \le n} (E_l - E_j)} \\ &= \sum_{l=0}^{n} \prod_{m=0}^{n} {}_{(m \neq l)} (E_l - E_m)^{-1}. \end{aligned}\right\} \quad \text{(B.18)}$$

However, $C(n)$ can be proved to be zero for all non-vanishing values of $(E_0, E_1 \ldots E_n)$ which are different from each other.

For the proof we consider the algebraic equation of degree $n \geq 1$:

$$f(x) = \sum_{l=0}^{n} \left\{ \prod_{m=0}^{n}{}_{(m \neq l)} \left(\frac{x - E_m}{E_l - E_m} \right) \right\} - 1 = 0. \qquad \text{(B.19)}$$

A factor $(x - E_k)$ is found in the numerators of all terms in the sum over l, except in the term with $l = k$. Therefore, substitution of $x = E_k$ leaves only the one term with $l = k$ which gives

$$f(E_k) = 1^n - 1 = 0. \qquad \text{(B.20)}$$

Thence, the algebraic equation (B.19) of degree n has at least $(n+1)$ roots $x = E_0, E_1, E_2 \cdots E_n$. This is possible only if the equation is an identity in x. Then, the coefficient of x^n must vanish. This coefficient is (for $n \geq 1$) just equal to $C(n)$ defined by (B.18). Hence, $C(n)$ and consequently N is zero for all non-vanishing and different values of the variables $(E_0, E_1, \cdots E_n)$. But, since $N(E_0, \cdots E_n)$ is a continuous function of these variables, N must then be zero for all values of $E_0, E_1 \cdots E_n$, which completes the proof of the equation (3.11) in Chapter III, i. e. Ψ_* is unitary if the series is so strongly convergent that the series Ψ_* and $\Psi_*^\dagger$ can be multiplied term by term.

C. Throughout this paper, k_0 means a particular set of values of the free particle variables k and quantities like $\langle k \mid Y \mid k_0 \rangle$ are thus matrices in k-space and $\mid k_0 \rangle$ is an eigenket of the k-variables corresponding to the eigenvalues k_0 (plane waves). On the other hand, k_0 is also used to label some of the stationary states (the scattering states) of the total system. For a reader who is accustomed to Dirac's notation, this may lead to confusion, since he might regard $\mid k_0 \rangle$ as identical with one of the scattering states $\mid n \rangle$ of the total system. To him, the matrix $\langle k \mid Y \mid k_0 \rangle$ in case of bound states may seem to be an incomplete matrix, i. e. a "non-square" matrix, as k labels a complete set of plane waves used in Fourier analysis of the field, while k_0 labels an incomplete set of functions. He may easily remedy this as follows.

First, complete $\langle k \mid Y \mid k_0 \rangle$ to a "square" matrix $\langle k \mid Y_m \mid n \rangle$ by adding columns of zeros: $\langle k \mid Y_m \mid k_0 \rangle = \langle k \mid Y \mid k_0 \rangle$; $\langle k \mid Y_m \mid r \rangle = 0$. The subscript m reminds us of the fact that Y_m is defined

in "mixed" (k and n) representations. In zeroth approximation, then, $\langle k | Y_m | n \rangle$ equals a matrix $\langle k | 1_m | n \rangle$, which consists of the unit matrix 1 in k-space bordered by colums of zeros:

$$\langle k | 1_m | k_0 \rangle = \delta(k - k_0); \quad \langle k | 1_m | r \rangle = 0. \quad \text{Thus,}$$
$$\langle k | Y_m | n \rangle = \langle k | 1_m | n \rangle + \langle k | Z_m | n \rangle.$$

The matrix 1_m obviously has the property $1_m \, 1_m^\dagger = 1$ in k-space, while $1_m^\dagger \, 1_m$ is a matrix in n-space with matrix elements

$$\langle k_0' | 1_m^\dagger 1_m | k_0'' \rangle = \langle k_0' | k_0'' \rangle, \langle k_0' | 1_m^\dagger 1_m | r'' \rangle$$
$$= \langle r' | 1_m^\dagger 1_m | k_0'' \rangle = \langle r' | 1_m^\dagger 1_m | r'' \rangle = 0$$

(even for $r' = r''$). We may then introduce matrices completely in k-space by $Y = Y_m 1_m^\dagger$ (thence, $Y^\dagger = 1_m \, Y_m^\dagger$). These matrices in k-space are the ones appearing in the text; for instance, Y, Z, B, Ψ, T, F, Ω, Γ, G, Q, P, W, R, K, S, 1 are matrices of this type, as well as their Hermitian conjugates $Y^\dagger$, $Z^\dagger$, etc.

These matrices, therefore, are obtained from the corresponding "mixed" matrices Y_m, $Y_m^\dagger$, etc., by first stripping the latter of their columns or rows of zeros, (thus changing $\langle k | Y_m | n \rangle$ into $\langle k | Y | k_0 \rangle$, $\langle n | Y_m^\dagger | k \rangle$ into $\langle k_0 | Y^\dagger | k \rangle$, or a product like $\langle n' | Y_m^\dagger Z_m | n'' \rangle$ into $\langle k_0' | Y^\dagger Z | k_0'' \rangle$, etc.), and then ignoring the difference in interpretation of the labels k and k_0, treating the latter as if it labels a complete set of plane waves just like k does.

D. It should be noted that, by assuming that each of the three sets $\langle k | Y | k_0 \rangle$ (with $Y = \Psi$ or Ω or Q) forms a set of functions of k sufficiently wide to express any scattering state linearly in terms of them, we did not assume that the $\langle k | Y | k_0 \rangle$ would form a complete set in which to express every function of k. That is, we did not preclude the existence of bound states. Nevertheless, for ensuring the existence of matrices X_1 and X_2 as described at the top of page 21, somewhat special assumptions had to be made about the lack of linear dependence of the differences between the sets of scattering states Ψ, Ω, and Q on the bound states ψ_r.

The necessity of these special assumptions for the validity of (2.48) can be made clearer by deriving the alternative form

which the relations (2.48) will take when these conditions are not fulfilled. In general, we find from (2.45), (2.47), and (2.40),

$$\Psi = \Psi S^\dagger S = \Psi \Psi^\dagger \Omega S = (1 - \sum_r \psi_r \psi_r^\dagger)\, \Omega S,$$

$$\Psi = \Psi\left(1 + \frac{iK}{2}\right)\left(1 + \frac{iK}{2}\right)^{-1} = \Psi \Psi^\dagger Q \left(1 + \frac{iK}{2}\right)^{-1}$$

$$= (1 - \sum_r \psi_r \psi_r^\dagger)\, Q \left(1 + \frac{iK}{2}\right)^{-1}.$$

Thence, also

$$\Psi S^\dagger = (1 - \sum_r \psi_r \psi_r^\dagger)\, \Omega, \qquad \Psi\left(1 + \frac{iK}{2}\right) = (1 - \sum_r \psi_r \psi_r^\dagger)\, Q.$$

These relations differ from the ones on page 21 by the occurrence of the factor

$$(1 - \sum_r \psi_r \psi_r^\dagger) = \Psi \Psi^\dagger.$$

From the discussions on pages 18—19, however, it is clear that this factor $\langle k' \mid \Psi \Psi^\dagger \mid k'' \rangle$ acts as the unit matrix whenever it acts on pure scattering states Ψ. Indeed,

$$(\Psi \Psi^\dagger)\, \Psi = \Psi\, (\Psi^\dagger \Psi) = \Psi \cdot 1 = \Psi,$$

by Eq. (2.34a). Our assumption made in words on page 20 now amounts to assuming that also

$$(\Psi \Psi^\dagger)\, \Omega = \Omega, \qquad (\Psi \Psi^\dagger)\, Q = Q.$$

In as far as this is the case, the above formulas reduce to the ones on page 21.

To the authors it seems quite possible that this assumption may turn out to be superfluous, that is, perhaps one can prove the automatic general validity of these equations. For various simple systems, such as the potential scattering of two particles, the mentioned equations are trivial indeed. However, for more

complicated systems, in which there may be bound states and scattering states belonging to the same degenerate energy level, we have not been able to find a general proof. As long as no proof of sufficient generality is available, we regard these equations as a somewhat special assumption, on which Eqs. (2.48), (5.24), and (9.26) are based.

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