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THE PROBLEM OF EXISTENCE OF A SCATTERING S-MATRIX. II

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It is shown that the S-operator cannot exist, but it is possible to define probabilities in momentum space by a careful transition to the limit. Our construction is quite independent of any asymptotic conditions upon the ingoing and outgoing fields.

In their efforts to derive an S-matrix from the quantum field theory, physicists used to start with a unitary operator $U(t_2, t_1)$ transforming the initial state $|i\rangle$ at the instan t_1 into the final state $|f\rangle$ at t_2 and performing a transition to the limit

$$S = \lim_{\substack{t_2\to\infty \\ t_1\to-\infty}} U(t_2, t_1) \tag{1}$$

where

$$|f\rangle = U(t_2, t_1)|i\rangle. \tag{2}$$

It is convenient to split the operator $U(t_2, t_1)$ as follows:

$$U_{21} \equiv U(t_2, t_1) = U(t_2, 0)\, U(0, t_1). \tag{3}$$

If $U(t, 0)$ is assumed to be of the form

$$U(t, 0) = e^{iH_0t}e^{-iHt} \tag{4}$$

then the matrix elements

$$\langle p''|U(t_2, t_1)|p'\rangle \tag{5}$$

are shown to denote probability amplitudes for obtaining, in a measurement at t_2, the eigenvalues p'', if the initial state at t_1 was an eigenstate to the eigenvalues p', where p means a complete set of observables commuting with the energy H_0 of the system of free particles. With the help of rather intuitive arguments it was argued that the limit transition (1) makes sense if performed cautiously, and that the eigenstates of H_0 go over asymptotically into the eigenstates of the total energy H belonging to the continuous part of its spectrum.

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However, the approach using such sophisticated arguments is mathematically dubious and physically incorrect.

First of all, the definition (2) of the scattering operator is ambiguous because it depends upon the choice of the Picture. In fact, using the Schrödinger Picture we get

$$U_{21}^{(S)} = e^{-iH(t_2-t_1)}, \tag{6}$$

while in the Heisenberg Picture it is nothing else but

$$U_{21}^{(H)} = 1 \tag{6'}$$

whereas only in the Interaction Picture

$$U_{21}^{(I)} = e^{iH_0t_2}e^{-iH(t_2-t_1)}e^{-iH_0t_1} \tag{6''}$$

is consistent with the usually assumed form (4) and is equivalent to Dyson's expression

$$U_{21}^{(D)} = T\exp\left(-i\int_{t_1}^{t_2} H'_{(I)}dt\right) \tag{7}$$

where $H'_{(I)}$ is the interaction energy expressed in the Interaction Picture and T is the operator of ordering in time.

In order to define the scattering amplitudes correctly we have to look more carefuly into the problem of probabilities for transitions between the initial and final states characterized by the eigenvalues ξ' and ξ'' respectively whereby ξ denotes a complete but arbitrary set of observables. Let us assume that the Schrödinger, Heisenberg, and Interaction Pictures coincide at $t = 0$ and denote the eigenstate to the eigenvalue ξ' at the instant $t = 0$ simply $|\xi'\rangle$. The ket vector, which is again an eigenvector to the same eigenvalue ξ' but for ξ measured at the time instant t, will be denoted by $|\xi', t\rangle$ (the corresponding bra by $\langle\xi', t|$). This must not be confused with the dynamical change of the state vector in the course of time! In order to avoid possible confusion we shall denote by $|t, \xi'\rangle$ (and $\langle t, \xi'|$) the state vector which has developed dynamically, in the course of time, from the initial $|\xi'\rangle$ and ceased to be the eigenvector to the eigenvalue ξ' unless ξ is a constant of motion. The probability amplitude of finding in a measurement performed at the instant t the eigenvalue ξ'', if the initial state was an eigenstate to the value ξ' at $t = 0$, is

$$a_{\xi''\xi'}(t) = \langle\xi'', t|t, \xi'\rangle. \tag{8}$$

This expression is quite general, independent of the Picture. Let us apply it first to the Heisenberg Picture. In this case the state vectors are dynamically time-independent, so that

$$|t, \xi'>_H = |\xi'>. \tag{9}$$

However, the operator $\xi(t)$ is time-dependent and $<\xi'', t|$ satisfies the eigenequation

$$<\xi'', t|\xi(t) = \xi''<\xi'', t| \tag{10}$$

or

$$<\xi'', t|e^{iHt}\xi e^{-iHt} = \xi''<\xi'', t|. \tag{10'}$$

Multiplying both sides of (10′) from the right by e^{iHt} we find that $<\xi'', t|e^{iHt}$ is an eigenvector of the operator $\check{\xi}$ (referred to the initial instant $t = 0$) to the eigenvalue ξ''. Hence,

$$<\xi'', t|e^{iHt} = <\xi''| \text{ or } <\xi'', t|_H = <\xi''|e^{-iHt}. \tag{11}$$

Introducing (9) and (11) into (8) we find

$$a_{\xi''\xi'}(t) = \langle\xi''|e^{-iHt}|\xi'\rangle. \tag{12}$$

In the Schrödinger Picture the situation is just reversed: the state vectors are dynamically time-dependent,

$$|t, \xi'>_S = e^{-iHt}|\xi'> \tag{13}$$

but, in contradistinction to the Heisenberg Picture, the vectors denoted by $|\xi'', t>$ become time-independent,

$$|\xi'', t>_S \equiv |\xi''> \tag{14}$$

because they satisfy the same eigenequation to the same eigenvalue of the same operator $\check{\xi}$ and, thus, can differ at most by an immaterial phase factor. Introducing (13) and (14) into (8) we find again the same result (12).

Let us check (12) also in the Interaction Picture. In this case the dynamical law is

$$|t, \xi'>_I = e^{iH_0t}e^{-iHt}|\xi'> \tag{15}$$

whereas $<\xi'', t|$ satisfies, ex definitione, the eigenequation

$$<\xi'', t|\check{\xi}_I(t) = \xi''<\xi'', t| \tag{16}$$

or

$$<\xi'', t|e^{iH_0t}\check{\xi}e^{-iH_0t} = \xi''<\xi'', t| \tag{16′}$$

whence it is inferred that

$$<\xi'', t|_{(I)} = <\xi''|e^{-iH_0t}. \tag{17}$$

Introducing (15) and (17) into (8) we get again (12).

In this way it is seen that it is the operator e^{-iHt} rather than $e^{iH_0t}e^{-iHt}$ which describes correctly the transition amplitudes. Consequently, it is rather the operator (6) and not (6″) which should be taken as a starting point for a correct derivation of the S-matrix.

Inasmuch as the operator (6″) does not define properly the probability amplitudes and, obviously, does not allow for the limit transition $t_2 \to \infty$, $t_1 \to -\infty$ the operator (7), being equivalent to (6″), does not allow it either. But these operators were defined in the Interaction Picture and the adequacy of the latter was put in doubt by several authors. Under such circumstances people tried to define the S-operator in the Heisenberg Picture. To this end the differential field equations valid in the Heisenberg Picture were replaced by integral equations expressing ψ as a sum of ψ^{in} and an integral involving the retarded Green function or as a sum of ψ^{out} and an integral involving the advanced Green function whereby the ingoing and outgoing fields mean free fields coinciding with the interacting field ψ asymptotically for $t \to -\infty$ and $t \to \infty$ respectively. The S-operator was defined as that transforming the ingoing into the outgoing fields

$$\psi^{\text{out}} = S^{-1} \psi^{\text{in}} S. \tag{18}$$

However, the integrals appearing in the integral equations possess only a meaning as limits of the corresponding integrals taken between t_1 and t_2 while ψ^{in} and ψ^{out} are to be understood as limits of free fields ψ^{t_1}, ψ^{t_2} coinciding (up to the first order derivative in the case of bosons) with the perturbed function ψ at the instants t_1 and t_2 respectively. Thus, the operator S must be understood as a limit

$$S = \lim_{\substack{t_1 \to -\infty \\ t_2 \to \infty}} U_{21} \tag{18'}$$

where

$$\psi^{t_2} = U_{21}^{-1} \psi^{t_1} U_{21}, \tag{18''}$$

if this limit transition exists.

However, a closed form for U_{21} may be obtained immediately without solving the integral field equations by iteration. In fact, since ψ^{t_1} and ψ^{t_2} are free fields, they satisfy

$$\psi^{t_1}(t_1) = e^{iH_0 t_1} \psi^{t_1}(0)\, e^{-iH_0 t_1} \tag{19}$$

$$\psi^{t_2}(t_2) = e^{iH_0 t_2} \psi^{t_2}(0)\, e^{-iH_0 t_2} \tag{19'}$$

and, from (18″)

$$\psi^{t_2}(0) = U_{21}^{-1} \psi^{t_1}(0)\, U_{21}. \tag{18'''}$$

Introducing (19) and (19′) into (18″) we get

$$e^{-iH_0 t_2} \psi^{t_2}(t_2) e^{iH_0 t_2} = U_{21}^{-1} e^{-iH_0 t_1} \psi^{t_1}(t_1) e^{iH_0 t_1} U_{21} \tag{20}$$

or

$$e^{-iH_0 t_2} \psi(t_2) e^{iH_0 t_2} = U_{21}^{-1} e^{-iH_0 t_1} \psi(t_1) e^{iH_0 t_1} U_{21} \tag{20'}$$

because $\psi^{t_2}(t_2)$ coincides with $\psi(t_2)$ and $\psi^{t_1}(t_1)$ with $\psi(t_1)$. In view of the dynamical relation

$$\psi(t_2) = e^{iH(t_2 - t_1)} \psi(t_1) e^{-iH(t_2 - t_1)} \tag{21}$$

the formula (20′) may be written in the form

$$e^{-iH_0 t_2} e^{iH(t_2 - t_1)} \psi(t_1) e^{-iH(t_2 - t_1)} e^{iH_0 t_2} = U_{21}^{-1} e^{-iH_0 t_1} \psi(t_1) e^{iH_0 t_1} U_{21} \tag{20''}$$

which yields

$$U_{21} = e^{-iH_0 t_1} e^{-iH(t_2 - t_1)} e^{iH_0 t_2}. \tag{22}$$

Comparing it with (6″) it is seen that U_{21} defined from integral equations valid in the Heisenberg Picture differs from (6″) obtained in the Interaction Picture merely by a unitary transformation and becomes identical with (6″) if the time interval is taken symmetrically with respect to zero ($t_2 = -t_1$). Thus, the operator U_{21} defined in the Heisenberg Picture is essentially the same as that defined in the Interaction Picture and presents the same difficulties: It denotes probability amplitudes in the momentum representation only and does not allow for a limit transition $t_2 \to \infty$, $t_1 \to -\infty$.

The mistake encountered so frequently in the literature, consisting in confusing the operators

$$S_{21} = e^{-iH(t_2-t_1)} \tag{23}$$

and

$$U_{21} = e^{iH_0 t_2}\, e^{-iH(t_2-t_1)}\, e^{-iH_0 t_1} \tag{23'}$$

came about from the fact that, usually, people started with discussing transitions between eigenstates of observables p commuting with the kinetic part of the energy H_0. In this and only this case both operators may be used equally well to compute probability amplitudes because the corresponding matrix elements differ only from each other by immaterial phase factors

$$\langle p''|U_{21}|p'\rangle = e^{iE_0''t_2}\langle p''|S_{21}|p'\rangle e^{-iE\,t_1} \tag{24}$$

and yield the same probabilities. However, it is unallowable to sandwich the operator U_{21} between states denoting wave packets, because wave packets do not possess a sharp value E_0. One forgets too often the fact that the matrix elements of U_{21} mean probability amplitudes only if sandwiched between eigenstates of H_0. This may be illustrated by the following very instructive example: Let us consider eigenstates of the total energy H. Using the correct operator S_{21} we get the correct result

$$\langle E'', \eta''|e^{-iHt}\,|E', \eta'\rangle = e^{-iE''t}\langle E'', \eta''|E', \eta'\rangle = 0 \tag{25}$$

if $E'' \neq E'$ or $\eta'' \neq \eta'$ (where η denotes the remaining observables specifying the state) because these states are stationary. On the other hand, by using the operator (4) and interpreting (wrongly) the corresponding matrix elements as probability amplitudes one gets

$$\langle E'', \eta''|e^{iH_0t}\, e^{-iHt}\,|E', \eta'\rangle = e^{-iE't}\langle E'', \eta''|e^{iH_0t}|E', \eta'\rangle \tag{25'}$$

which usually is different from zero for $E'' \neq E'$ because H_0 does not commute with H. In view of such a result people used to speculate that the apparent non-conservation of energy is explicable in terms of the fourth uncertainty relation $\Delta E \cdot \Delta t \sim h$ where Δt means a finite interval between the two measurements. Such speculations only show ignorance as to the meaning and role of the fourth uncertainly relation in quantum theory.

On the other hand, the form S_{21} being valid for arbitrary initial and final states, nothing prevents us from sandwiching it between state vectors representing wave packets separated spatially at the initial and final instants, *i.e.* to describe with the help of S_{21} genuine scattering processes.

The correct transition operator may be written in the form

$$S(t, 0) = e^{-iH_0t}\, T \exp\left(-i \int_0^t H_I'\, dt'\right) \tag{26}$$

and developed into a power series in terms of the interaction Hamiltonian H_I^0. Thus, a perturbative expansion is still possible if H' may be regarded as "small'.

Mere inspection of the formula (23) for S_{21} or (26) for $S(t, 0)$ shows that these operators exist only for a finite time interval and the limit transition $t_1 \to -\infty$ $t_2 \to \infty$ is impossible. The S-operator does not exist and no mathematical tricks with the limit transitions can help it.

Nevertheless, probabilities can exist if we start with wave packets. In this case the amplitudes are

$$a_{\tilde{p}''\tilde{p}'} = \int dp'' \int dp' a^*(p'') e^{-iE_0''t_2} \langle p'' | T \exp\left(-i \int_{t_1}^{t_2} dt H_I'\right) | p' \rangle e^{iE_0't_1} a(p'). \tag{27}$$

Due to the appearance in (27) of the exponential factors $e^{\pm iE_0 t}$ (which were missing in the usual approach starting with (3) and (4)) the integrations over a finite interval ΔE_0 yield the necessary damping for large values t_2 and $-t_1$ because the packets overlap only during a time interval of the order

$$\Delta t \cdot \Delta E_0 \sim h. \tag{28}$$

Consequently, the limit transitions $t_2 \to \infty$, $t_1 \to -\infty$ are allowed for the squared absolute values of (27). The limit transition $\Delta E_0 \to 0$ is also allowed in (22) provided we keep the inequality

$$(t_2 - t_1)\, \Delta E_0 \gg \mathrm{h}, \tag{29}$$

otherwise we would run into contradictions: either obtain a meaningless result or a triviality $S = 1$.

The above described approach is completely independent of any assumption about the asymptotic properties of the ingoing and outgoing waves.