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The Delay Time Operator for Simple Scattering Systems

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1. Introduction

In this paper we shall give a new discussion of the concept of "delay-time" associated with a collision process, and its relation to the phase shift in a single channel scattering process.

This concept and a special case of the associated relation appeared in the published literature first in a paper by WIGNER [1] who in turn refers to an earlier unpublished thesis by Eisenbud for a fuller discussion of it.

The concept was generalized by F. T. SMITH [2] to the "delay-time matrix" for a general multichannel process and he obtained generalized relations connecting this matrix with the S-matrix.

We shall reformulate this concept here in the context of the scattering theory of JAUCH [3] which avoids the use of eigenfunction expansions. This enables us to give a definition of the delay-operator Q for more general scattering systems (for which the eigenfunction expansion need not be valid) and to determine at the same time the condition of validity for the above mentioned relation between the operator Q and the scattering operator S.

In this paper we shall do this for a simple scattering system, reserving the more general multichannel case for a later publication.

The general relation between the operators Q and S was also derived with an operator method by GOLDBERGER and WATSON [4], however we have found their method unsuited for a mathematically rigorous treatment. In fact we did not succeed in determining the conditions of validity of their formal manipulations. For this reason we have adopted a different procedure designed to simplify the mathematical aspects of the problem and to permit a derivation of this relation with meaningful concepts.

We were motivated by the aim to determine the weakest possible conditions under which the definition of the operator Q makes sense and is related to the S-operator in the manner given by the above mentioned authors. It is clear that the asymptotic condition and the completeness condition (these are the conditions I and II of reference [3]) must be satisfied. We have found that in order to obtain the desired relation a further condition is needed which expresses a regularity property of the wave operators. In all applications known to us this condition is in fact satisfied, but it is worth emphasizing that this third condition seems not derivable from the other two.

Finally we should mention that the relation between delay-operator Q and the S-operator are independent of the representations and can therefore be expressed in principle as a general functional relations between these two operators. We have found it not very convenient to do so. The most convenient form is obtained by using the spectral representation of these operators with respect to a complete set of commuting operators which contains among them the kinetic energy H_0 since this spectral representation can be proved to be quite generally valid [5] (in contradistinction to the eigenfunction expansion which exists only under restrictive special conditions) the generality of the relation is assured in spite of the special form under which it is expressed.

2. Basic definitions

We shall be dealing with a simple scattering system represented for instance by the scattering of a particle by a fixed center of force. Such a system is described by the two operators H_0 and $H = H_0 + V$, where $H_0 = (1/2\,\mu)\,p^2$ represents the kinetic energy of the particle and V the interaction which produces the scattering.

The exact form of H_0 is not essential for the following, so that for instance the relativistic form $\sqrt{p^2 + \mu^2}$ for H_0 would be equally admissible. Neither is it essential that we consider the three-dimensional case for which $p^2 = p_1^2 + p_2^2 + p_3^2$ where p_i are the components of the orthogonal directions. We can also include one- or two-dimensional scattering problems with similar results. We shall however discuss explicitly primarily the three-dimensional non-relativistic case in order not to obscure the discussion with too much generality.

For a simple scattering system the operator V satisfies the asymptotic condition of ref. [3] which guarantees the existence of the limits

$$\Omega_\pm = s - \lim_{t \to \mp\infty} V_t^*\, U_t \tag{1}$$

with $U_t = e^{-iH_0 t}$, $V_t = e^{-iHt}$, thereby defining the two wave operators $\Omega_\pm$. They satisfy the intertwining relation $H_0\,\Omega_\pm = \Omega_\pm\,H$ and $\Omega_-^*\,\Omega_- = \Omega_+^*\,\Omega_+ = I$, $\Omega_-\,\Omega_-^* = \Omega_+\,\Omega_+^*$. With their help one defines the S-operator: $S = \Omega_-^*\,\Omega_+$.

The evolution of a pure state during the scattering process is given by $\psi_t = V_t\,\psi$, where $\psi \equiv \psi_0$ is the wave function of that state at the time $t = 0$. To every such ψ one can associate two other states $\varphi_{in} = \Omega_+^*\,\psi$ and $\varphi_{out} = \Omega_-^*\,\psi$, so that $\varphi_{out} = S\,\varphi_{in}$.

Let us now consider a sphere of radius r centered at the scattering center, and denote by P_r the projection operator associated with the proposition that the particle is inside this sphere. Thus in the Schrödinger representation the operator P_r acts on wave functions $\varphi(\boldsymbol{x})$ in the following manner

$$(P_r\,\varphi)\,(\boldsymbol{x}) = \begin{cases} \varphi(\boldsymbol{x}) & \text{for } \;|\,\boldsymbol{x}\,| \leqslant r \\ 0 & \text{for } \;|\,\boldsymbol{x}\,| > r \end{cases}. \tag{2}$$

For any given state φ the quantity $(\varphi,\,P,\,\varphi) \equiv \langle P_r\rangle_\varphi$ represents the probability of finding the particle inside the sphere of radius r. We may therefore interprete

$$T_r(\psi) \equiv \int_{-\infty}^{+\infty} \langle P_r\rangle_{\psi_t}\,dt \tag{3}$$

as the average total time spent by the particle inside the sphere of radius r, during the scattering process described by the wave function ψ. This time is in general finite for finite r and any ψ in the common range of the wave operators $\Omega_\pm$. It also tends to ∞ if r tends to ∞.

We can introduce for comparison another quantity

$$T_r(\varphi) \equiv \int_{-\infty}^{+\infty} \langle P_r \rangle_{\varphi_t} \, dt \tag{4}$$

where $\varphi_t = U_t \varphi$ and φ is either one of the two state vectors φ_{in} or φ_{out} (which we need not specify here, since subsequently the choice will turn out to be irrelevant).

The quantity (4) has similar properties as (3) and it may be interpreted as the average time spent by a *free* particle inside the sphere of radius r.

The difference between these two quantities (3) and (4) represents then the time delay associated with a state φ and the sphere of radius r. We write for it

$$\Delta T_r(\varphi) \equiv \int_{-\infty}^{+\infty} (\langle P_r \rangle_{V_t \Omega_+ \varphi} - \langle P_r \rangle_{U_t \varphi}) \, dt \tag{5}$$

where we have written $\psi = \Omega_+ \varphi$ (thereby choosing $\varphi = \varphi_{in}$).

The quantity (5) still depends on the radius r of the chosen sphere but it may approach a finite limit as r tends to ∞. The study of examples has shown that this limit may not actually exist due to the presence of oscillating terms even in cases where one would expect for physical reasons the notion of delay-time to be well defined. Such oscillating terms can be suppressed easily by using not the straightforward limit of $\Delta T_r(\varphi)$ for $r \to \infty$, but the "average limit" $1/r \int_r^{2r} dr \, \Delta T_r(\varphi)$ for $r \to \infty$.

The particular form of this averaging of the limit is not essential, we could use just as well any of a number of averaging procedures which can be shown to give all the same result.

By these considerations we are led to define the quantity

$$\langle Q \rangle_\varphi \equiv \lim_{r \to \infty} \frac{1}{r} \int_r^{2r} dr \int_{-\infty}^{+\infty} dt \, (\langle P_r \rangle_{V_t \Omega_+ \varphi} - \langle P_r \rangle_{U_t \varphi}) \, . \tag{6}$$

It is not difficult to verify that the right hand side of (6) defines a bounded symmetrical sesquilinear functional on the entire space $\mathcal{H}$. By the use of standard theorems every such functional defines a unique, bounded, self adjoint operator Q, as we have already anticipated with the notation

$$\langle Q \rangle_\varphi \equiv (\varphi, Q \varphi) \, .$$

We may therefore give a well defined meaning to the expression

$$Q \equiv \lim_{r \to \infty} \frac{1}{r} \int_r^{2r} dr \int_{-\infty}^{+\infty} dt \, U_t^* \, (\Omega_+^* \, P_r \, \Omega_+ - P_r) \, U_t \tag{7}$$

as a bounded linear operator which we consider the definition of the "delay-operator" Q.

3. Elementary properties of Q

Let A be a bounded linear operator, U_t a continuous unitary group and assume that the integral

$$B = \int_{-\infty}^{+\infty} dt\, U_t^* \, A \, U_t$$

exists for all φ in a Hilbert space. Let τ be a fixed real number. Then we have

$$B\, U_\tau = \int_{-\infty}^{+\infty} dt\, U_t^* \, A \, U_{t+\tau} \,.$$

Changing the variable of integration we obtain

$$B\, U_\tau = \int_{-\infty}^{+\infty} dt\, U_{t-\tau}^* \, A \, U_t = U_\tau \, B \,.$$

Thus B commutes with all U_τ and hence with all functions of the U_τ, hence with the generator G of U_τ as well as with its spectral projections.

Let us now consider the spectral representation [5] of the operator Q with respect to a complete set of commuting observables of which we may choose G together with an arbitrary commuting set X.

According to the theorem on the spectral representation [5], we can associate with any $\varphi \in \mathcal{H}$ a complex function $\langle g\, \lambda \mid \varphi)$ of the spectral variables g, λ of G and X, square integrable with respect to a uniquely defined measure class μ, so that [6]

$$(\varphi, \psi) = \int (\varphi \mid g\, \lambda\rangle \, \langle g\, \lambda \mid \psi)\, d\mu$$

where

$$(\varphi \mid g\, \lambda\rangle = \langle g\, \lambda \mid \varphi)^* \,. \tag{8}$$

Any operator such as B which commutes with G can be written in "diagonal form", that is we may define a family of operators $B(g)$ operating for each g on square integrable functions $\varphi_g(\lambda)$ of the variable λ with respect to a uniquely defined measure class which we denote by $d\lambda$, such that

$$\begin{aligned} \langle g\, \lambda \mid B\varphi\,) &= (B(g)\, \varphi_g)\, (\lambda) \\ \varphi_g(\lambda) &= \langle g\, \lambda \mid \varphi) \,. \end{aligned} \tag{9}$$

If we suppose in addition that the operator A is a well-defined integral operator in the spectral representation $\{g, \lambda\}$ whose kernels $\langle g\, \lambda \mid A \mid g'\, \lambda'\rangle$ are for any fixed g, λ, λ' good testfunctions with respect to the distribution $\delta(g - g')$ the following calculation takes on a well defined sense:

$$\begin{aligned} \langle g\, \lambda \mid B\varphi) &= \int dg'\, d\lambda' \int_{-\infty}^{+\infty} dt\, \langle g\, \lambda \mid U_t^* \, A \, U_t \mid g'\, \lambda'\rangle \, \langle g'\, \lambda' \mid \varphi) \\ &= \int dg'\, d\lambda' \int_{-\infty}^{+\infty} dt\, e^{-i(g-g')t} \, \langle g\, \lambda \mid A \mid g'\, \lambda'\rangle \, \langle g'\, \lambda' \mid \varphi) \\ &= \int d\lambda'\, 2\pi \, \langle g\, \lambda \mid A \mid g\, \lambda'\rangle \, \langle g\, \lambda' \mid \varphi) \,, \end{aligned}$$

and we obtain the result:

$$\left.\begin{aligned} \langle g\,\lambda \mid B \mid g'\,\lambda' \rangle &= \delta\,(g-g')\,\langle \lambda \mid B(g) \mid \lambda' \rangle \\ \text{with} \qquad \langle \lambda \mid B(g) \mid \lambda' \rangle &= 2\,\pi\,\langle g\,\lambda \mid A \mid g\,\lambda' \rangle\,. \end{aligned}\right\} \tag{10}$$

We may now apply this description to the definition (7) of Q. Identifying G with H_0 and A with $\Omega_+^*\,P_r\,\Omega_+ - P_r$ for each r and then passing to the limit $r \to \infty$ we obtain first the result: Q commutes with H_0.

Consider furthermore the spectral representation with respect to H_0 and an arbitrary set X of commuting observables, or, what is often more convenient: with respect to $K = \sqrt{2\,\mu\,H_0}$ and X (denoting the spectral variables $\{\omega, \lambda\}$ in the first and by $\{k, \lambda\}$ in the second case). If the kernels $\langle k\,\lambda \mid \Omega_r^*\,P_r\,\Omega_+ - P_r \mid k\,\lambda' \rangle$ are well-defined and if they are, for fixed variables k, λ, λ', good functions in k' (this property will always be assumed in the sequal) Equations (10) read

$$\begin{aligned} \langle k\,\lambda \mid Q \mid k'\,\lambda' \rangle &= \delta\,(k-k')\,\langle \lambda \mid Q(k) \mid \lambda' \rangle \\ \langle \lambda \mid Q(k) \mid \lambda' \rangle &= \lim_{r\to\infty} \frac{1}{r} \int_r^{2r} dr\, \frac{2\,\pi\,dk}{d\omega}\, \langle k\,\lambda \mid \Omega_+^*\,P_r\,\Omega_+ - P_r \mid k\,\lambda' \rangle\,. \end{aligned} \tag{11}$$

We say $Q(k)$ are operators "on the energy shell".

It is well known that the S-operator is also an operator on the energy shell and therefore also has the form

$$\langle k\,\lambda \mid S \mid k'\,\lambda' \rangle = \delta\,(k-k')\,\langle \lambda \mid S(k) \mid \lambda' \rangle\,.$$

Our aim is to derive a general relation between the S-operator and the Q-operator which can be expressed by the equation

$$\langle \lambda \mid Q(k) \mid \lambda' \rangle = \frac{1}{i}\,\frac{dk}{d\omega} \int d\lambda'\,\langle \lambda' \mid S^*(k) \mid \lambda \rangle\,\frac{d}{dk}\,\langle \lambda' \mid S(k) \mid \lambda \rangle \qquad \left[\omega = \frac{k^2}{2\,\mu}\right]. \tag{12}$$

In the equivalent operator form this equation may be written as

$$\boxed{Q(k) = -\,i\,\frac{d}{d\omega}\,\ln\,S(k)} \tag{13}$$

which corresponds to Equ. (285a) in ref. [4].

In the particular case that $S(k)$ is diagonal in the variables λ it has the form $S(k) = e^{2\,i\,\delta(k)} \cdot I$ where $\delta(k)$ defines the phase shift. The relation (12) resp. (13) takes then the form

$$Q(k) = 2\,\frac{d\,\delta(k)}{d\omega} \tag{14}$$

in which it was originally obtained.

4. An example

Before we proceed to a formal theorem and its proof we illustrate the main ideas in the derivation of relation (13) with an example. We choose for this purpose a one-dimensional scattering problem. In this case the S-matrix as well as the Q-matrix are two-dimensional matrices since the "energy-shell" consist of exactly two points which correspond to the two directions of motion on the line. This circumstance enables us to simplify the notation a little by choosing for the variable k not the variable in the spectrum of the operator $K = \sqrt{2\,\mu\, H_0}$ but of the operator p instead. This k extends then over the entire real axis and it is just the Fouriertransform of the position variable x. The S-matrix is then formally one-dimensional and we can suppress the variable λ entirely.

In this representation the operator P_r (which now is interpreted as the projection onto the segment $(-r, +r)$) becomes

$$\langle k \mid P_r \mid k' \rangle = \int_{-r}^{+r} dx \, \langle k \mid x \rangle \, \langle x \mid k' \rangle \,. \tag{15}$$

Here

$$\langle k \mid x \rangle = \frac{1}{\sqrt{2\,\pi}} \, e^{i k x} \tag{16}$$

is the kernel of the Fouriertransformation.

By substituting (16) into (15) we find

$$\langle k \mid P_r \mid k' \rangle = \frac{1}{\pi} \, \frac{\sin r \, (k' - k)}{k' - k} \,. \tag{17}$$

For a dense set of sufficient regular functions $\varphi(k)$ from a linear test function space we have the limiting relation

$$\lim_{r \to \infty} \int_{-\infty}^{+\infty} dk' \, \frac{1}{\pi} \, \frac{\sin r \, (k' - k)}{k' - k} \, \varphi(k') = \varphi(k) \,, \tag{18}$$

which represents the more general relation (valid for all $\varphi \in \mathfrak{H}$)

$$\underset{r \to \infty}{\text{l.i.m.}} \langle k \mid P_r \, \varphi) = \langle k \mid \varphi) \,. \tag{19}$$

Both of these relations are consequences of the operator relation

$$s\text{—}\lim_{r \to \infty} P_r = I \,. \tag{20}$$

The operators Ω_+ for instance satisfy an integral equation which can be written in the following way [7]:

$$\langle k \mid \Omega_+ \mid k' \rangle = \delta\,(k - k') + \frac{\langle k \mid V\, \Omega^+ \mid k' \rangle}{\omega' - \omega + i\,0} \,. \tag{21}$$

This form shows that $\langle k \mid \Omega_+ \mid k' \rangle$ is always a distribution (which contains a δ-function) however $\langle k \mid V\, \Omega_+ \mid k' \rangle$ may be and in fact is in all problems of physical interest a bona fide integral kernel applicable to a dense set of $\varphi(k)$ in L^2.

The S-matrix itself (as a two-dimensional matrix) may be written in the following way: We introduce indices r, s which may assume values ± 1, and denote $\sqrt{k^2}$ by $\mid k \mid$. Then

$$\langle r \mid S\,(\mid k \mid) \mid s \rangle = \delta_{rs} - 2\pi i \, \frac{d \mid k \mid}{d\omega} \, \langle \mid k \mid r \left| V\, \Omega_+ \right| \mid k \mid s \rangle \,. \tag{22}$$

If we insert the spectral representation of P_r into the expression (7) in order to obtain the spectral representation of Q we find ourselves quickly in the presence of terms of the form

$$\fint_{-\infty}^{+\infty} dk' \langle k \mid P_r \mid k' \rangle \frac{\langle k' \mid V \Omega^+ \mid k \rangle}{(k'+k)\,(k'-k)} . \tag{23}$$

We are interested in the limit $r \to \infty$ (before or after the averaging over r, as the case may be) and look to Equ. (18) to give us the answer. But we find (18) not applicable since the function which multiplies $\langle k \mid P_r \mid k' \rangle$ in (23) is singular at the point $k = k'$ and it is therefore not a good testfunction for a sequence of distributions $\langle k \mid P_r \mid k' \rangle$ tending to $\delta\,(k - k')$. Consequently we write the expression (23) in the form

$$\fint_{-\infty}^{+\infty} dk' \, \frac{\langle k \mid P_r \mid k' \rangle}{k'-k} \, \frac{\langle k' \mid V \Omega^+ \mid k \rangle}{k'+k} \tag{23}$$

and study the limit ($r \to \infty$) of the kernel

$$\frac{\langle k \mid P_r \mid k' \rangle}{k'-k} .$$

In the present example this amounts to studying the limit of the integral

$$\fint_{-\infty}^{+\infty} dk' \, \frac{1}{\pi} \, \frac{\sin r\,(k'-k)}{(k'-k)^2} \, \varphi(k') \tag{23}$$

as $r \to \infty$ with $\varphi(k)$ in a testfunction space of infinitely differentiable functions.

Under these conditions we can develop $\varphi(k')$ according to

$$\varphi(k') = \varphi(k) + (k' - k)\, \varphi'\,(k + \theta\,(k' - k)) \tag{24}$$

with

$$0 \leqslant \theta < 1$$

so that (23) becomes

$$\fint_{-\infty}^{+\infty} dk' \, \frac{1}{\pi} \, \frac{\sin r\,(k'-k)}{(k'-k)^2} \, \varphi(k')$$

$$= \varphi(k) \fint_{-\infty}^{+\infty} \frac{1}{\pi} \, \frac{\sin r\,(k'-k)}{(k'-k)^2} + \int_{-\infty}^{+\infty} dk' \, \frac{1}{\pi} \, \frac{\sin r\,(k'-k)}{k'-k} \, \varphi'\,(k + \theta\,(k' - k)) \tag{25}$$

The first term on the right of (25) is identically zero for all r because of the antisymmetry of the integrand. The second term can be evaluated in the limit by using formula (18) (with φ' replacing φ) and all the higher order terms vanish in the limit $r \to \infty$. Consequently we find

$$\lim_{r \to \infty} \frac{1}{\pi} \fint_{-\infty}^{+\infty} \frac{\sin r\,(k'-k)}{(k'-k)^2} \, \varphi(k') = \varphi'(k) . \tag{26}$$

A relation of this kind explains in a qualitative way the appearance of the *derivative* of $S(k)$ in the relation (13). At the same time it is made plausible that the condition $P_r \to I$ is *not* sufficient for the validity of relation (13). The kernels $\langle k \mid V \Omega_+ \mid k' \rangle$ resp. $\langle k \mid \Omega_+^* V \mid k' \rangle$ should belong to a testfunction space on which

(a) The kernels $\langle k \mid P_r \mid k' \rangle$ converge to $\delta(k - k')$ as $r \to \infty$

(b) The kernels $P(1/k' - k) \langle k \mid P_r \mid k' \rangle$ converge to $-\delta'(k - k')$ as $r \to \infty$, where convergence is defined as the numerical convergence of the definite integrals

$$\int \langle k \mid P_r \mid k' \rangle \frac{\langle k' \mid V \Omega_+ \mid k \rangle}{k' + k} dk'$$

respectively

$$\fint \frac{\langle k \mid P_r \mid k' \rangle}{k' - k} \frac{\langle k' \mid V \Omega_+ \mid k \rangle}{k' + k} dk' .$$

These remarks may suffice for the motivations of the conditions under which we can affirm the theorem of the next section.

5. The main theorem

Theorem: Let the kernels $\langle k \lambda \mid P_r \mid k' \lambda' \rangle$ be distributions on a testfunction space $\mathcal{A}$ containing at least the integral kernels $\langle k \lambda \mid V \Omega_+ \mid k' \lambda' \rangle$ and $\langle k \lambda \mid \Omega_-^* V \mid k' \lambda' \rangle$ considered as functions of $k' \lambda'$ (for fixed k, λ) or as functions of k, λ (for fixed k', λ'), and suppose that the following assumptions hold for the distributions:

(a) $$\langle k \lambda \mid P_r \mid k' \lambda' \rangle \xrightarrow{r \to \infty} \delta(k - k') \, \delta(\lambda - \lambda')$$

(b) $$P\left(\frac{1}{k' - k}\right) \langle k \lambda \mid P_r \mid k' \lambda' \rangle \xrightarrow{r \to \infty} -\delta'(k - k') \, \delta(\lambda - \lambda')$$

(c) $$\lim_{r \to \infty} \frac{1}{r} \int_r^{2r} dr \, \langle k \lambda \mid P_r \mid k \lambda' \rangle = 0 \qquad [\lambda \neq \lambda']$$

then the following relation holds

$$\int d\lambda'' \langle \lambda \mid S(k) \mid \lambda'' \rangle \langle \lambda'' \mid Q(k) \mid \lambda' \rangle \equiv \langle \lambda \mid (SQ)(k) \mid \lambda' \rangle = \frac{1}{i} \frac{dk}{d\omega} \frac{d}{dk} \langle \lambda \mid S(k) \mid \lambda' \rangle . \tag{27}$$

Proof: We remark first that the relation (27) is easily seen to be equivalent with either (12) or (13), by virtue of the unitarity of the S-matrix.

Multiplying (7) from the left by $S = \Omega_-^* \Omega_+$, then applying the relations $\Omega_+^* \Omega_+ = I$ and $[S, U_t] = 0$ and finally writing out the spectral representation in the variables $\{k, \lambda\}$ according to (11) we obtain the expression

$$\langle \lambda \mid (S\,Q)(k) \mid \lambda' \rangle = \lim_{r \to \infty} \frac{1}{r} \int_{2r}^{r} dr \, \frac{2\pi \, dk}{d\omega} \langle k\lambda \mid \Omega_-^* [P_r, \Omega_+] \mid k \lambda' \rangle . \tag{28}$$

We now split the wave operators according to $\Omega_\pm = I + T_\pm$ to transform the claimed relation (27) into

$$\lim_{r\to\infty}\frac{1}{r}\int_r^{2r} dr\,\frac{2\pi\,dk}{d\omega}\,\langle k\,\lambda\mid[P_r, T_+]\mid k\,\lambda'\rangle + \lim_{r\to\infty}\frac{1}{r}\int_r^{2r} dr\,\frac{2\pi\,dk}{d\omega}\,\langle k\,\lambda\mid T_-^*[P_r, T_+]\mid k\,\lambda'\rangle$$
$$= \frac{1}{i}\,\frac{dk}{d\omega}\,\frac{d}{dk}\,\langle\lambda\mid R(k)\mid\lambda'\rangle\,. \tag{29}$$

We have replaced S by $R = S - I$ on the righthand side of (27) since I is independent of k and therefore gives zero upon differentiation with respect to k.

Further we carry out the following substitutions which are standard formulae of scattering theory [7]

$$\left.\begin{aligned}
\langle k\,\lambda\mid T_+\mid k'\,\lambda'\rangle &= \frac{\langle k\lambda\mid V\,\Omega_+\mid k'\,\lambda'\rangle}{\omega'-\omega+i\,0}\\
\langle k\,\lambda\mid T_-^*\mid k'\,\lambda'\rangle &= -\frac{\langle k\lambda\mid \Omega_-^*\,V\mid k'\,\lambda'\rangle}{\omega'-\omega-i\,0}\\
\langle k\,\lambda\mid R\mid k'\,\lambda'\rangle &= \delta\,(k-k')\,\langle\lambda\mid R(k)\mid\lambda'\rangle\\
\langle\lambda\mid R(k)\mid\lambda'\rangle &= -\,2\,\pi\,i\,\frac{dk}{d\omega}\,\langle k\,\lambda\mid V\,\Omega_+\mid k\,\lambda'\rangle\,.
\end{aligned}\right\} \tag{30}$$

Let us examine the first part on the left hand side of Equ. (27). The variables λ are only trivially involved and we can omit writing them in the following

$$\frac{2\pi\,dk}{d\omega}\,\langle k\mid[P_r, T_+]\mid k\rangle = \frac{2\pi\,dk}{d\omega}\left\{\int_0^\infty dk'\,\langle k\mid P_r\mid k'\rangle\,\langle k'\mid V\,\Omega_+\mid k\rangle\,\frac{1}{\omega-\omega'+i\,0}\right.$$
$$\left.-\int_0^\infty dk'\,\langle k\mid V\,\Omega_+\mid k'\rangle\,\langle k'\mid P_r\mid k\rangle\,\frac{1}{\omega'-\omega+i\,0}\right\}.$$

By using the formulae

$$\frac{1}{x-i\,0} = P\Big(\frac{1}{x}\Big) + \pi i\,\delta(x)\,;\;\frac{1}{x+i\,0} = P\Big(\frac{1}{x}\Big) - \pi i\,\delta(x)$$

and

$$P\Big(\frac{1}{\omega'-\omega}\Big) = \frac{dk}{d\omega}\Big(\frac{1}{k'-k} - \frac{1}{k'+k}\Big)$$

we obtain

$$\langle k\mid[\,P_r, T_+]\mid k\rangle = \int_0^\infty dk'\left\{\langle k\mid P_r\mid k'\rangle\,\langle k'\mid V\,\Omega_+\mid k\rangle\right.$$
$$\times\,\frac{dk}{d\omega}\left[P\Big(\frac{1}{k'-k}\Big) - \frac{1}{k'+k} + \pi i\,\delta(k'-k)\right] + \int_0^\infty dk'\,\langle k\mid V\,\Omega_+\mid k'\rangle\,\langle k'\mid P_r\mid k\rangle$$
$$\left.\times\,\frac{dk}{d\omega}\left[P\Big(\frac{1}{k'-k}\Big) - \frac{1}{k'+k} - \pi\,i\,\delta\,(k'-k)\right]\right\}.$$

First we note that in the limit $r \to \infty$ the terms containing $1/(k' + k)$ will just give $1/2\,k$ by property (a) of the hypotheses. Then the terms containing $P(1/(k' - k))$ can be evaluated in the limit $r \to \infty$ using property (b) of the hypotheses. Finally the terms containing the δ-functions read

$$\frac{i\pi}{2k} \int d\lambda'' \{\langle k\lambda \mid V\Omega_+ \mid k\lambda''\rangle \langle k\lambda'' \mid P_r \mid k\lambda'\rangle - \langle k\lambda \mid P_r \mid k\lambda''\rangle \langle k\lambda'' \mid V\Omega_+ \mid k\lambda'\rangle\}$$

(where we have restored the variable λ) and they vanish when the averaging $1/r \int_r^{2r} dr$ in (7) and the property (c) of the hypotheses are applied. (Without this averaging the above expression would not be uniquely defined and an explicit calculation e.g. in the example (17) would lead to the undertemined expression $\infty - \infty$.) The result is

$$\begin{aligned}
&\lim_{r\to\infty} \frac{1}{r} \int_r^{2r} dr\, \langle k \mid [P_r, T_+] \mid k\rangle \\
&= \frac{\partial}{\partial k'} \langle k' \mid V\Omega_+ \mid k\rangle_{k'=k} \frac{dk}{d\omega} + \frac{\partial}{\partial k'} \langle k \mid V\Omega_+ \mid k'\rangle_{k'=k} \frac{dk}{d\omega} - \frac{1}{k} \langle k \mid V\Omega_+ \mid k\rangle \frac{dk}{d\omega} \\
&= \frac{dk}{d\omega} \left(\frac{d}{dk} \langle k \mid V\Omega_+ \mid k\rangle - \frac{1}{k} \langle k \mid V\Omega_+ \mid k\rangle\right).
\end{aligned}$$

Since $d\omega/dk = k/\mu$ it follows that $d/dk\,(dk/d\omega) = -\,dk/d\omega\; 1/k$ and therefore

$$\frac{d}{dk} R(k) = -\,2\pi i \frac{dk}{d\omega} \left(\frac{d}{dk} \langle k \mid V\Omega_+ \mid k\rangle - \frac{1}{k} \langle k \mid V\Omega_+ \mid k\rangle\right)$$

so that

$$\lim_{r\to\infty} \frac{2\pi\, dk}{d\omega} \langle k \mid [P_r, T_+] \mid k\rangle = \frac{1}{i} \frac{dk}{d\omega} \frac{d}{dk} R(k)\,. \tag{31}$$

By restoring the variables λ at their proper place we obtain the relation

$$\lim_{r\to\infty} \frac{1}{r} \int_r^{2r} dr\, \frac{2\pi\, dk}{d\omega} \langle k\lambda \mid [P_r, T_+]\, k\lambda'\rangle = \frac{1}{i} \frac{dk}{d\omega} \frac{d}{dk} \langle\lambda \mid R(k) \mid \lambda'\rangle\,. \tag{32}$$

This shows that the entire contribution (29) must come from the first term on the left. Thus the relation (29) and with it the theorem is proved if we can prove that the second term on the left of (29) is zero. That is we must prove the relation

$$\lim_{r\to\infty} \frac{1}{r} \int_r^{2r} dr\, \frac{2\pi\, dk}{d\omega} \langle k\lambda \mid T_-^* \,[P_r, T_+] \mid k\lambda'\rangle = 0\,. \tag{33}$$

This expression contains three kinds of terms, characterized by the number of δ-functions contained in them. A straight forward calculation shows that the terms which contain at least one δ-function exactly cancel each other. The remaining terms containing the two principal value parts read (without unessential constants and averaging)

$$\lim_{r\to\infty} \fint_0^\infty \frac{dk'}{k'-k}\, f_r(k, k') \quad \text{with} \quad f_r(k, k')$$

$$= \frac{\langle k \mid \Omega^* V \mid k' \rangle}{k'+k} \fint_0^\infty dk'' \left[\frac{\langle k' \mid P_s \mid k'' \rangle}{k-k''} \frac{\langle k'' \mid V \Omega_+ \mid k \rangle}{k''+k} - \frac{\langle k' \mid V \Omega_+ \mid k'' \rangle}{k'+k''} \frac{\langle k'' \mid P_r \mid k \rangle}{k''-k'} \right]. \quad (34)$$

Now we note from (a) that the functions $f_r(k, k')$ converge to zero uniformly in any interval of k' which does not contain k, while for $k' = k$ they converge to a number different from zero according to (b) and the convergence is not uniform in the neighborhood of k. In any interval of uniform convergence limit and integral may be interchanged in (34) whence

$$\lim_{r\to\infty} \fint_{2k}^\infty \frac{dk'}{k'-k}\, f_r(k, k') = \fint_{2k}^\infty \frac{dk'}{k'-k} \lim_{r\to\infty} f_r(k, k') = 0 \quad (35)$$

and the integration $\int_0^\infty$ in (34) may be replaced by $\int_0^{2k}$.

In this remaining integral the limit cannot be taken inside since the convergence of f_r is not uniform. But we may split f_r into a symmetric and an antisymmetric part in k' as follows:

$$f_r(k, k') = S f_r(k, k') + A f_r(k, k')$$
$$S f_r(k, k + \varkappa) = S f_r(k, k - \varkappa)$$
$$A f_r(k, k + \varkappa) = - A f_r(k, k - \varkappa)$$

and discuss the truncated integral (34) separately for the two parts.

From the symmetry of $S f_r$ with respect to the integration domain it follows immediately that (34) vanishes. The antisymmetric part $A f_r$ tends to zero uniformly on the entire k'-halfaxis, and the argument used in (35) shows that (34) vanishes as well. This proves the theorem.

6. Example: The elastic scattering of a spinless particle

In this last section we shall show that for the case of a spinless particle in three-dimensional space the three conditions (a), (b) and (c) of the preceding section are satisfied for any testfunction which is sufficiently differentiable.

In this example we may choose for the complete set of commuting observables the operators $K = \sqrt{2\mu H_0}$, L^2 and L_3, with the spectral variables $\{k, l, m\}$.

Let us calculate

$$\langle k\, l\, m \mid P_r \mid k'\, l'\, m' \rangle = \int_{\varrho \leq r} \langle k\, l\, m \mid \varrho\, \vartheta\, \varphi \rangle \langle \varrho\, \vartheta\, \varphi \mid k'\, l'\, m' \rangle$$

$$= \int_0^r d\varrho\, \varrho^2 \int_0^\pi d\vartheta \sin\vartheta \int_0^{2\pi} d\varphi\, \chi_l^*(k\varrho)\, Y_{lm}^*(\vartheta, \varphi)\, \chi_{l'}(k'\varrho)\, Y_{l'm'}(\vartheta, \varphi)$$

where

$$\chi_l(kr) = \sqrt{\frac{k}{r}}\; J_{l+1/2}(kr)\,.$$

Integration over the angles gives

$$\langle k\, l\, m \mid P_r \mid k'\, l'\, m' \rangle = \delta_{ll'}\, \delta_{mm'}\, \langle k \mid P_r \mid k' \rangle$$

with

$$\langle k \mid P_r \mid k' \rangle = \int_0^r d\varrho\, \varrho^2\, \chi_l(k\,\varrho)\, \chi_l(k'\,\varrho)\,.$$

The last integral can be referred to Lommels integral [8] and can be evaluated in the following form:

$$\langle k \mid P_r \mid k' \rangle = \frac{r^2}{k^2 - k'^2} \left\{ \chi_l(kr)\, \frac{d}{dr}\, \chi_l(k'\,r) - \frac{d}{dr}\, \chi_l(kr)\, \chi_l(k'\,r) \right\}. \tag{36}$$

We may develop this expression into an asymptotic powers series in $1/r$ by using

$$\chi_l(kr) = \sqrt{\frac{2}{\pi}} \left(\frac{1}{r} \sin\left(kr - \frac{\pi\, l}{2}\right) + \frac{1}{r}\, O\left(\frac{1}{kr}\right)\right).$$

We are now prepared to prove property (a). Since the higher order terms in $1/r$ give zero in the limit $r \to \infty$ we may write $\langle k \mid P_r \mid k' \rangle$

$$\simeq \frac{2}{\pi} \frac{r^2}{k^2 - k'^2} \left\{ \frac{k'}{r^2} \sin\left(kr - \frac{\pi\, l}{2}\right) \cos\left(k'r - \frac{\pi\, l}{2}\right) - \frac{k}{r^2} \sin\left(k'r - \frac{\pi\, l}{2}\right) \cos\left(kr - \frac{\pi\, l}{2}\right)\right\}$$

$$\simeq \frac{1}{\pi} \left\{ \frac{\sin r\,(k' - k)}{k' - k} - (-1)^l\, \frac{\sin\, r\;(k' + k)}{k' + k} \right\}. \tag{37}$$

The second term tends for $r \to \infty$ to a δ-function with support at the point $k = -k'$ and thus does not contribute anything while the first term tends to $\delta\,(k' - k)$ (cf. section 3). This verifies property (a).

Let us now verify property (b) that is

$$\lim_{r\to\infty} \fint_0^\infty \frac{dk'}{k' - k}\, \langle k \mid P_r \mid k' \rangle\, \varphi(k') = \varphi'(k) \tag{38}$$

for any testfunction $\varphi(k)$. It suffices to verify this relation for leading terms (37) in the asymptotic expansion of $\langle k \mid P_r \mid k' \rangle$ the other terms being zero in the limit $r \to \infty$.

We note that because property (a) is verified we may decompose the integral (38) into two parts one on the interval $(0,\, 2\, k)$ and the other on $(2\, k,\, \infty)$. The second integral is then seen to vanish in the limit $r \to \infty$ because of (a).

By a reasoning which duplicates word for word that which lead us to Equ. (26) we verify that a necessary and sufficient condition for the truth of Equ. (38) is

$$\lim_{r\to\infty} \fint_0^{2k} \frac{\langle k \mid P_r \mid k' \rangle}{k' - k}\, dk' = 0 \qquad [k > 0]\,. \tag{39}$$

This property results by direct evaluation for the leading term (37) of the asymptotic expansion of the kernel $\langle k \mid P_r \mid k' \rangle$. For the other terms it is true because these terms are of order $1/r$ or less and therefore tend to zero with $r \to \infty$. This verifies property (b).

Finally property (c) follows easily from the explicit form (35) of the leading term in $\langle k \mid P_r \mid k' \rangle$. Thus our three conditions for the validity of the proof of the main theorem are verified in this case.

7. Conclusion

The main result of this paper is the derivation of the relation (13) between the delay-time operator Q and the scattering operator S. This relation is valid for all simple scattering systems for which the wave operators $\Omega_\pm$ satisfy the regularity conditions that $V \Omega_\pm$ and $\Omega^*_- V$ have in the k-representations integral kernels which in both variables are functions from a testfunction space for which the conditions (a), (b) and (c) are valid. The last three conditions are valid for elementary particles with or without spin if the testfunction space contains for instance infinitely differentiable functions only. We have shown this in section (6) for spinless particles.

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