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Time-Delay in Scattering Processes

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Abstract. The relation between time-delay and the phase-shift operator is derived in the context of the time-dependent scattering theory for simple (single channel) scattering systems.

The sufficient conditions on the interaction under which this relation can be established in a mathematical correct manner are formulated and the precise sense in which this relation can be interpreted is discussed.

The results obtained here generalize and unify various partial results previously published on this subject.

1. Introduction

We shall reconsider in this paper the relation between the time-delay during a scattering process and the rate of change of the phase shift with the energy.

This relation has been obtained by more or less heuristic reasoning a long time ago. We are of the opinion that the physical and mathematical significance of this relation merits a more detailed, more general and more rigorous derivation.

Physically speaking the relation is a quantitative expression of the plausible fact that a particle which spends a long time in the neighborhood of a scattering center suffers a stronger scattering than one which passes through the region of the scatterer in a very short time.

This relationship is exhibited very clearly in resonance scattering processes in nuclear physics, for instance. It is known that in the neighborhood of a resonance the scattering passes through a maximum which can be very accurately described by a Breit-Wigner type formula. The effective width of this formula Γ is roughly the inverse of the lifetime of the resonant state.

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There is no essential distinction between a resonant state with a practically unmeasurable delay-time and the formation of a metastable state. It is therefore desirable to develope a formalism which permits a unified description af all degrees of resonance scattering and which is applicable for the entire range of values for the lifetime of an unstable particle.

Considered from a different point of view the relationship which we shall establish is a precise mathematical derivation of what is sometimes loosely expressed as the uncertainty relation between time and energy in the context of a scattering process. If ΔT is the time-delay and $\Delta E = \Gamma$ the width of the energy of a resonance, then this uncertainty relation says that $\Delta T \, \Delta E \simeq 1$ (in units $\hbar = c = 1$). The derivations of such an uncertainty relation are notoriously unsatisfactory and it is one of the side results of this paper to clarify this point.

The time-delay during a scattering process is a quantity which is in principle measurable, although there are very few experimental situations where such a measurement is feasible. But if the measurement is feasible then it may be considered a complementary piece of information over and above the differential scattering cross-section.

It is known that a knowledge of the differential cross-section even in its energy dependence does not suffice for the determination of the scattering amplitude and the phase-shifts. A supplementary and independent physical datum, like the time-delay may therefore be quite useful for the reconstruction of the scattering amplitude from the scattering data. If one considers an individual spherical wave in a spherically symmetrical scattering problem the time-delay can be shown to be proportional to the derivative of the phase-shift with respect to the energy, so that a measurement of the time-delay would constitute a measurement of the rate of change of the phase-shift with energy.

This relation between the variation of the phase-shift and the time-delay seems to have been noted first by Eisenbud in an unpublished thesis. Many books on scattering theory give a simple 'derivation' of this relationship with a reasoning somewhat as follows:

Let the amplitude of an incoming spherical wave (multiplied with the distance from the scattering center) be described by a radial wave packet of the form

$$\int_0^\infty \varphi(k)\, e^{-i(kr+\omega t)}\, dk \quad \text{with} \quad \omega \sim \frac{k^2}{2\,m} \quad (\text{in units } \hbar = c = 1)$$

and $\varphi(k)$ be a continuous and square integrable function peaked around a value k_0. This wave packet moves in the radial direction in x-space with a velocity which can be calculated approximately as follows:

The integral will be appreciably different from zero, only if the phase of the exponential function is stationary near the value $k = k_0$. This means

$$0 \sim \frac{d}{dk}(k\,r + \omega\,t)\Big|_{k=k_0} = r + t\frac{d\omega}{dk}\Big|_{k=k_0}.$$

This shows that for $t < 0$ the wave packet moves towards the center of scattering with a velocity $v_0 = (d\omega/dk)\,|_{k=k_0}$.

The scattered radial wave will appear for $t > 0$ and it has the form

$$\int \varphi(k)\, e^{2i\delta + ikr - i\omega t}\, dk\ ,$$

where δ is the phase-shift for that particular spherical wave.

With the same argument as before we obtain the values of r and t for which this integral is appreciably different from zero from the formula

$$0 \sim r - v_0\, t + 2 \left.\frac{d\delta}{dk}\right|_{k = k_0}$$

or

$$r = v_0(t - \varDelta t)\ ,$$

where

$$\varDelta t = 2 \left.\frac{d\delta}{d\omega}\right|_{k = k_0}$$

is the time-delay.

While this 'derivation' may suffice for a physical visualization of the time-delay formula, it can of course not be considered as sufficient for establishing it.

The actual relationship between time-delay and scattering amplitude requires first of all a mathematically more precise definition of time-delay. It is then found that this relation is of much more general validity than the special case considered here. The actual proof of this relationship requires considerable mathematical work some of which is of intrinsic interest of its own as pure mathematics.

A general derivation of this relation was attempted by Goldberger and Watson in their book on scattering theory [1]. Their formal treatment gives some valuable clues for a general approach to the proof but it does not constitute a proof of their theorem.

A mathematically correct proof of the theorem was attempted by Jauch and Marchand [2]. Their result was not entirely satisfactory either since in the course of the proof some hypothesis are needed of a mathematical character which have no good physical justification and which are actually stronger than necessary.

We therefore reexamine this problem once again and develope here an entirely different mathematically more powerful technique for obtaining the desired result. We shall restrict ourselves here to the simple (one channel) scattering system, although the theorem has been generalized to the multichannel case [3].

Many of the mathematical results that we shall obtain here are known in one way or another either by formal non-rigorous methods or rigorously but sometimes in a different context. In the latter category, we mention in particular the remarkable work by Krein and by Birman. Actually by using certain of their results some of our work has been shortened.

In spite of rather heavy mathematics we try, insofar as possible, to maintain the physical interpretation. This is especially useful for the motivation of some of the basic definitions which are needed at the outset.

Much of the mathematical technique that we shall need is based on the theory of the resolvent operators corresponding to the two unitary groups U_t and V_t which describe the 'free' and the 'true' evolution of the system.

One of the major difficulties of a technical nature is caused by the need for establishing relationships for certain limits of operators, and operators on the energy shell. This is the physicists term for the component operators which appear in a direct integral representation with respect to the 'free' Hamiltonian $\overset{0}{H}$. While we are not sure that we have found the best way of handling these difficulties, we believe the results are correct but may perhaps be established with greater ease by using more powerful methods than we know.

During all of this work we shall be concerned with operators in a separable Hilbert space $\mathscr{H}$. A simple scattering system is characterized by two self-adjoint operators $\overset{0}{H}$ and H, on a common dense domain $D \equiv D_{\overset{0}{H}} = D_H$ of definition, which satisfy the (strong) asymptotic condition. The associated unitary groups will be denoted by U_t and V_t. The common resolvent set $\varrho(H) \cap \varrho(\overset{0}{H})$ is an open subset of the complex plane which includes all z with $\operatorname{Im} z \neq 0$. The resolvents will be denoted by $\overset{0}{R}_z = (\overset{0}{H} - z \cdot I)^{-1}$ and $R_z = (H - z \cdot I)^{-1}$. An important quantity in the following will be the difference of the resolvants $D_z = R_z - \overset{0}{R}_z$. In much of this work we shall assume that D_z is a trace class operator $\mathscr{L}_1(\mathscr{H})$.

The set $\mathscr{L}_1$ is defined as the set of operators T with the property that $|T| \equiv \sqrt{T^* T}$ has a finite trace, so that for any complete orthonormal set of vectors the sum $Tr\,|T| \equiv \Sigma(\varphi_r, |T|\,\varphi_r)$ exists and is finite. It is then independent of the set of the vectors and its value is the trace norm $\|T\|_1 = Tr\,|T|$ of the operator T.

Much of the work will be concerned with the passage from the abstract Hilbert space $\mathscr{H}$ to a particular representation in the form of a direct integral $\int \oplus \mathscr{H}_\lambda \, d\lambda$ consisting of functions $\lambda \to \psi_\lambda \in \mathscr{H}_0$ from λ to vectors in a fixed Hilbert space $\mathscr{H}_0$ and satisfying

$$\int_\Lambda \|\psi_\lambda\|_0^2 \, d\lambda < \infty \,, \quad \text{where} \quad \|\cdot\|_0$$

denotes the norm in $\mathscr{H}_0$ and the integral is extended over the spectrum of $\overset{0}{H}$. In all of the following Λ will be identified with the positive real axis $\boldsymbol{R}^+$, which is the case for a non-relativistic scattering system. In this space every bounded operator T which commutes with $\overset{0}{H}$ has also a component representation $T = \{T_\lambda\}$ where T_λ is an operator in $\mathscr{H}_0$. All these component representations are only defined up to sets of measure zero with respect to Lebesgue measure on Λ, and so are all of their properties. For instance the T_λ are bounded in $\mathscr{H}_0$ for almost every λ.

Our first task will be the definition of the delay time with respect to a sphere of radius r whose center coincides with the scattering center. This we shall do in Section 2. We shall then study in the following Section the passage to the limit $r \to \infty$. And finally in the last Section we shall establish the relation of this expression with the crossection.

2. The Time-Delay for a Finite Sphere

A simple scattering system is characterized by two one-parameter continuous unitary groups U_t, V_t, representing physically the evolution of the states for a free particle and a particle moving in the force field of a scattering center. These two groups satisfy the asymptotic condition

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

We shall write $\varphi_t = U_t \varphi$, $\psi_t = V_t \psi$ and for every fixed unit vector ψ we can define two 'asymptotic states' φ^{in} and φ^{out} defined by

$$\lim_{t \to -\infty} \| \psi_t - \varphi_t^{in} \| = 0 ,$$

$$\lim_{t \to +\infty} \| \psi_t - \varphi_t^{out} \| = 0 . \tag{2}$$

The equivalence of (2) with (1) is easily verified by setting

$$\Omega_+ \varphi^{in} = \psi = \Omega_- \varphi^{out} . \tag{3}$$

One can show that the operators $\Omega_\pm$ are isometries ($\Omega_\pm^* \Omega_\pm = I$) and for simple scattering systems they have identical range, so that the operator

$$S = \Omega_-^* \Omega_+ \tag{4}$$

is unitary. It satisfies $\varphi^{out} = S \varphi^{in}$.

Let us now consider a sphere of radius r in $\boldsymbol{R}^3$ and the projection operator P_r in the Hilbert space $L^2(\boldsymbol{R}^3)$ defined by

$$(P_r \psi)(x) = \begin{cases} \psi(x) & \text{for } |x| < r , \\ 0 & \text{for } |x| \geq r . \end{cases} \tag{5}$$

If the normalized element $\psi(x) \in L^2(\boldsymbol{R}^3)$ represents the (pure) state of a particle then we can express the probability of finding the particle inside this sphere by the formula

$$(\psi, P_r \psi) \equiv \int_{|x| < r} | \psi(x) |^2 \, dx . \tag{6}$$

Suppose now that the system undergoes an evolution, so that the state becomes a function of time $\psi_t = V_t \psi$. Then this probability will also become time-dependent and it is given at each instant by

$$(\psi_t, P_r \psi_t) = (\psi, V_t^* P_r V_t \psi) . \tag{7}$$

We can then define the *mean time* spent by the particle in the sphere by

$$T = \int_{-\infty}^{\infty} (\psi_t, P_r \psi_t) \, dt . \tag{8}$$

It is not obvious that this integral should be finite. For instance it certainly is not if there exists a point eigenvalue λ_0 for the generator H of $V_t = e^{-iHt}$. If ψ is an eigenfunction corresponding to such an eigenvalue, then $\psi_t = e^{-i\lambda_0 t}\,\psi$ and therefore $(\psi_t, P_r\,\psi_t) = (\psi, P_r\,\psi)$ is independent of t. It is for this reason that such states are called bound states.

The situation is different if ψ is a scattering state, that is if it is a vector in the common range of $\Omega_{\pm}$. But even in this case it is not known whether the integral (8) is finite for all such ψ. So we shall develope the theory independently of this assumption.

The expression (8) should be compared with a similar expression constructed with the states $\varphi_t^{in} = U_t\,\varphi^{in}$. We call the corresponding expression

$$T^{in} = \int_{-\infty}^{\infty} (\varphi_t^{in}, P_r\,\varphi_t^{in})\,dt \tag{9}$$

and we define the *time-delay* for the sphere of radius r the quantity $\Delta T_r \equiv T - T^{in}$, or

$$\Delta T_r = \int_{-\infty}^{\infty} [(\psi_t, P_r\,\psi_t) - (\varphi_t^{in}, P_r\,\varphi_t^{in})]\,dt\,. \tag{10}$$

We consider this as the diagonal element of a bilinear functional by writing $\varphi = \varphi^{in}$, $\psi = \Omega\,\varphi$ ($\Omega = \Omega_+$) and obtain in this notation the fundamental quantity

$$\Delta T_r = \int_{-\infty}^{\infty} (\varphi, U_t^*[\Omega^*\,P_r\,\Omega - P_r]\,U_t\,\varphi)\,dt\,. \tag{11}$$

In the passage from (10) to (11) we have used the intertwining relation

$$V_t\,\Omega = \Omega\,U_t\,. \tag{12}$$

The time delay ΔT_r as defined in (11) has the inconvenience that it depends on r, the radius of the sphere considered in x-space. This radius is an entirely unphysical parameter and should be eliminated. This means we should study the limit as $r \to \infty$. This limit is quite delicate and most of the next section is devoted to its study. It is obvious that we cannot simply put $r = \infty$ inside the integral, since this would make the expression vanish. We also found it impossible to prove the existence of the limit for all φ and in fact there exist counter examples.

In Ref. [2] we have used a stronger kind of limit and proved its existence for a certain subclass of scattering systems. This subclass was singled out by purely mathematical considerations and has no physical significance. This was the unsatisfactory part in that paper.

In this paper we shall proceed therefore differently. It will be shown that (11) represents a bilinear form on a certain dense linear subset of $\mathscr{H}$ which is diagonal in the spectral representation. The diagonal elements are then shown to be represented by trace class (and hence bounded) operators on the energy shell for almost all $\lambda \in \Lambda = \overset{0}{\mathrm{sp}H}$. Furthermore the limit of these operators exists as $r \to \infty$ (again almost everywhere, of course).

This result cannot be established with the hypothesis of the strong asymptotic condition alone. The condition that we need is however the weakest known sufficient condition on the existence of the asymptotic condition and it admits all the physically interesting cases of short range interactions.

3. The Delay-Time on the Energy Shell

We are ultimately interested in the delay-time for the infinite region. The passage to the limit $r \to \infty$ poses some technical problems. We prepare in this section the appropriate handling of these problems by introducing another representation of the time-delay.

The expression which we have obtained for the time-delay in the state φ was

$$\Delta T_r = (\varphi, T_r \varphi) ,$$

where formally the 'operator' T_r could be written as

$$T_r = \int_{-\infty}^{\infty} U_t^* [\Omega^* P_r \Omega - P_r] U_t \, dt . \qquad \text{`(11)'}$$

The integral over dt has the consequence that the 'operator' T_r commutes with $\overset{0}{H}$, that is, in the spectral representation with respect to $\overset{0}{E}_\lambda$ it should be a diagonal operator. It is interesting that although T_r is in general not definable as a bona fide operator, these diagonal operators are so definable and their properties can be established relatively easily. In particular the limit $r \to \infty$ can be carried out for the time-delay operators on the energy-shell as we shall show in the next section.

In order to obtain the maximum information from the expression '(11)' it is convenient to study first expressions of the type '(11)' with the bracket replaced by an operator Γ of trace class. The integrand of '(11)' needs not be (and in general is not) of trace class, but such an operator is obtainable from (11) by the artifice of multiplying '(11)' from the right and from the left with the resolvent operator $\overset{0}{R}_z$.

The transition to the energy-shell will be accomplished with the help of two theorems to be given in this section. In the application we shall identify Γ with

$$\Gamma = \overset{0}{R}{}_z^* [\Omega^* P_r \Omega - P_r] \overset{0}{R}_z ,$$

where $z \in \varrho(H) \cap \varrho(\overset{0}{H})$ is any fixed complex number in the common resolvent set of H and $\overset{0}{H}$.

Let us first of all verify that the operator Γ is trace class. It is based on two elementary facts concerning these operators which we mention here for convenience.

(i) $\Gamma \in \mathscr{L}_1$ if and only if $\Gamma = A\,B$; $A, B \in \mathscr{L}_2$ where $\mathscr{L}_2$ denotes the Hilbert-Schmidt operators.
(ii) If $A \in \mathscr{L}_2$, $B \in \mathscr{L}$ (bounded operators) then $A\,B \in \mathscr{L}_2$ and $B\,A \in \mathscr{L}_2$.
(iii) If $A \in \mathscr{L}_2$ then $A^* \in \mathscr{L}_2$.

Let us examine the first term in the expression for Γ. After the use of the intertwining relation $\Omega \overset{0}{R}_z = R_z \Omega$ it becomes $\Omega^* R_z^* P_r R_z \Omega$. Because of (i), (ii) and (iii) we need only verify that $P_r R_z \in \mathscr{L}_2$. Since by the resolvent identity $R_z = \overset{0}{R}_z(I - V \overset{0}{R}_z)$ if $D_H = D_H^0 = D$ (see introduction) and $I - V \overset{0}{R}_z$ is bounded, it suffices to prove only that $P_r \overset{0}{R}_z \in \mathscr{L}_2(\mathscr{H})$. This also suffices for the second term.

In order to verify this we consider $\overset{0}{R}_z$ in the x-representation where it takes the form of an integral operator:

$$\langle x \mid \overset{0}{R}_z \mid y \rangle = \frac{1}{4\pi} \frac{e^{i\sqrt{z}\,|x-y|}}{|x-y|}\,; \quad (\operatorname{Im} \sqrt{z} > 0)\,.$$

If $\chi_r(x)$ is the characteristic function of the sphere of radius r then the operator $P_r \overset{0}{R}_z$ has the kernel

$$\langle x \mid P_r \overset{0}{R}_z \mid y \rangle = \frac{1}{4\pi} \chi_r(x) \frac{e^{i\sqrt{z}\,|x-y|}}{|x-y|}\,.$$

Now

$$\iint |\langle x \mid P_r \overset{0}{R}_z \mid y \rangle|^2 \, d^3x\, d^3y$$

$$= \frac{1}{(4\pi)^2} \iint \left| \chi_r(x) \frac{e^{i\sqrt{z}\,|x-y|}}{|x-y|} \right|^2 d^3x\, d^3y < \infty\,.$$

This proves that $P_r \overset{0}{R}_z$ is Hilbert-Schmidt and thus completes the proof that Γ is trace-class.

Let us now return to the expression '(11)' and assume that Γ is trace-class. For such operators we have the

Theorem 1:

Let $U_t = e^{-i\overset{0}{H}t}$ be a unitary group with the self-adjoint generator $\overset{0}{H}$ and the absolutely continuous spectrum Λ, and Γ an arbitrary trace class operator. Then there exists a dense set $\mathscr{D} \subset \mathscr{H}$ such that $\forall\, f, g \in \mathscr{D}$

$$G[f, g] = \int_{-\infty}^{\infty} (f, U_t^* \Gamma U_t g)\, dt \tag{13}$$

exists and defines a sesquilinear functional on $\mathscr{D} \times \mathscr{D}$ (that is linear with respect to g and antilinear with respect to f).

If $f_\lambda, g_\lambda \in \mathscr{H}_0$ are the components of f respectively g in the direct integral representation with respect to spectral family of $\overset{0}{H}$, then

$$G[f, g] = \int_{\Lambda} (f_\lambda, G_\lambda g_\lambda)\, d\lambda\,, \tag{14}$$

where G_λ is an essentially unique family of trace-class operators in $\mathscr{H}_0$ for almost all λ and

$$\int_\Lambda Tr_0\, G_\lambda\, d\lambda = 2\,\pi\, Tr\,\Gamma\,. \tag{15}$$

Finally

$$\int_\Lambda \|\, G_\lambda \|_{01}\, d\lambda \leq 2\,\pi\, \|\,\Gamma\,\|_1\,. \tag{16}$$

In these formulae $(.\,,.)_0$ denotes the scalar product, Tr_0 the trace, and $\|\,.\,\|_{01}$ the trace norm in $\mathscr{H}_0$.

Formula (15) has a fairly obvious content. Speaking loosely, the integral over t will introduce with respect to the spectral variables $2\,\pi$ times the δ-function. If the trace is identified with the diagonal integral then what is left is a family of operators on the diagonal defined by $G = 2\,\pi\,\langle\lambda\,|\,\Gamma\,|\,\lambda\rangle$ and the total trace is the integral of the traces on the diagonal, that is formula (15).

A correct proof of Theorem 1 requires considerable more work and we shall give it in Appendix A in order not to break the main line of the argument.

Theorem 1 permits us now to obtain sufficiently strong statements concerning an operator of type '(11)' where the bracket of the integrand is not of trace class. In order to do this we introduce a dense set $\mathscr{D}_0$ which is contained in the set $\mathscr{D}$ of theorem 1. This set is defined as

$$\mathscr{D}_0 = \{f \in \mathscr{H} \mid \|\,f_\lambda\,\|_0 \ \text{ has compact support, and } \ \operatorname*{ess.sup}_{\lambda\in\Lambda} \|\,f_\lambda\,\|_0 < \infty\}\,. \tag{17}$$

We shall use the notation somewhat loosely in the sense that we denote with the same letter $\mathscr{D}_0$ the subset in the direct integral $\mathscr{G} = \int \oplus\, \mathscr{H}_\lambda\, d\lambda$ and in the abstract space $\mathscr{H}$ which is isomorphic with it.

For all $f,\, g \in \mathscr{D}_0$ we define the sesquilinear form

$$\int_{-\infty}^{\infty} (f,\, U_t^*\, Tr\, U_t\, g)\, dt \equiv B_r[f,\, g] \tag{18}$$

and we have the following

Theorem 2:

If $D_H = D_H^0$ and $r < \infty$ the integral (18) exists and represents a finite sesquilinear form on $\mathscr{D}_0 \times \mathscr{D}_0$. There exists an essentially unique (that is up to sets of measure zero) family of trace class operators Q_λ^r in $\mathscr{H}_0$ defined for *a. a.* $\lambda \in \Lambda$, such that

$$\int_{-\infty}^{\infty} (f,\, U_t^*\, Tr\, U_t\, g)\, dt = \int_\Lambda d\lambda (f_\lambda,\, Q_\lambda^r\, g_\lambda)_0 \;\forall\, f,\, g \in \mathscr{D}_0\,. \tag{19}$$

The family Q^r_λ has the additional properties

(i) $$2\pi\, T_r \overset{0}{R}{}^*_z\, T_r \overset{0}{R}_z = \int_\Lambda \frac{Tr_0\, Q^r_\lambda}{|\lambda - z|^2}\, d\lambda \;\; \forall\; z \in \varrho(H) \cap \varrho(\overset{0}{H}),$$

(ii) $$\int_\Lambda \frac{|T_{r_0}\, Q^r_\lambda|}{|\lambda - z|^2}\, d\lambda \le 2\pi\, \| \overset{0}{R}{}^*_z\, Tr\, \overset{0}{R}_z \|_1 .$$

Proof of Theorem 2:

If $f \in \mathscr{D}_0$ then $f \in D_H = D^0_H$ and $(\overset{0}{H} - z) f \equiv f_z \in \mathscr{D}_0 \subset \mathscr{D}$ for any fixed $z \in \varrho(H) \cap \varrho(\overset{0}{H})$.

Let $\{f^z_\lambda\}$ be the representation of f_z in the direct integral representation, so that

$$f^z_\lambda = (\lambda - z)\, f_\lambda .$$

It follows that

$$B_r[f, g] = \int_{-\infty}^{\infty} (f, U^*_t\, Tr\, U_t\, g)\, dt = \int_{-\infty}^{\infty} dt (f_z, U^*_t\, \overset{0}{R}{}^*_z\, Tr\, \overset{0}{R}_z\, U_t\, g_z)$$

satisfies the hypothesis of theorem 1. Let $G^r_\lambda(z)$ be the essentially unique family of trace class operators and define

$$Q^r_\lambda = |\lambda - z|^2\, G^r_\lambda(z) .$$

It follows then that Q^r_λ is trace class in $\mathscr{H}_0$ and that

$$B_r[f, g] = \int_\Lambda (f_\lambda, Q^r_\lambda\, g_\lambda)_0\, d\lambda .$$

This shows that Q^r_λ is independent of z and this proves the first part of Theorem 2.

Again from Theorem 1, we obtain

$$2\pi\, Tr\, \overset{0}{R}{}^*_z\, Tr\, \overset{0}{R}_z = \int_\Lambda d\lambda\, T_{r_0}\, G^r_\lambda(z) = \int_\Lambda d\lambda \frac{Tr_0\, Q^r_\lambda}{|\lambda - z|^2}$$

and

$$\int_\Lambda \frac{|Tr_0\, Q^r_\lambda|}{|\lambda - z|^2}\, d\lambda \le 2\pi\, \| \overset{0}{R}{}^*_z\, Tr\, \overset{0}{R}_z \|_1 \tag{20}$$

and this proves the remaining statements of Theorem 2.

The operators Q^r_λ may be interpreted as the delay-time operators on the energy shell. The trace of Q^r_λ (which is finite) represents, loosely speaking, the total time delay for wave packets with energy concentrated in the region λ.

The next point to be investigated is the behavior of these operators in the limit $r \to \infty$.

4. The Delay Time for Infinite Space

Let r_n ($n = 1, 2, 3, \ldots$) be an increasing sequence of positive numbers which tend to infinity as $n \to \infty$. For each such sequence we have an associated sequence of operators $Q_\lambda^n \equiv Q_\lambda^{r_n}$ defined, almost everywhere in $[0, \infty]$, by the two theorems of the previous section. We want to study the limit of $Tr_0\, Q_\lambda^n \equiv \tau_n(\lambda)$ as $n \to \infty$.

It is not to be expected that this limit should exist for every value $\lambda \in \Lambda$. The physical reason for this is easy to see: It may occur that the operator H has point eigenvalues λ_i embedded in the continuous part of the spectrum. For $\lambda = \lambda_i$ we should expect that $\tau_n(\lambda_i) \to \infty$ as $n \to \infty$, because, the eigenvalue λ_i being a stationary state would lead to an infinitely long scattering time.

As far as we could determine it is not known whether the condition $D_z \in \mathscr{L}_1$, suffices to rule out such eigenvalues.

Besides this assumption we shall make another one, viz. that the projection P whose range are the stationary states has finite dimensions. This means there are only a finite number of bound states with finite multiplicity.

If the potential function V is spherically symmetric, then one can for instance, use Bargmann's bound viz.

$$n_l(V) \le \frac{1}{2\,l+1} \int_0^\infty r \mid V(r) \mid dr\,,$$

where $n_l(V)$ is the number of negative energy bound-states of angular momentum l (not counting multiplicity). Since $n_l(V)$ must be an integer or zero, this shows the finiteness of the number of negative energy bound stages provided the integral on the right hand side exists.

As for positive energy bound states, we can only say that in most physical potential scattering problem one does not encounter them.

The foregoing remarks lead one to expect that the convergence of $\tau_n(\lambda)$ for $n \to \infty$ could be expressed as a convergence in the sense of a distribution. With this we mean the following:

Let $\mathscr{D}$ be the class of test functions of the variable λ and let $f(\lambda) \in \mathscr{D}$. Then we may calculate

$$\int \tau_n(\lambda)\, f(\lambda)\, d\lambda = f_n\,.$$

The convergence of $\tau_n(\lambda)$ may then be expressed as follows: There exists a distribution $\tau(\lambda)$ such that

$$f = \lim_{n \to \infty} f_n = \int_\Lambda \tau(\lambda)\, f(\lambda)\, d\lambda\,.$$

The distribution will consist of two parts, one which involves δ-functions at the values $\lambda = \lambda_i$ corresponding to the stationary states and another continuous part arising from the variation of the S-operator with λ.

In order to express this second part we recall the fact that the S-operator is diagonal in the spectral representation of $\overset{0}{H}$ since it commutes with $\overset{0}{H}$. Hence it is represented by a family S_λ of unitary operators on the energyshell.

It is convenient to define the *phaseshift operator* Δ_λ by setting

$$S_\lambda = e^{2i\Delta_\lambda}.$$

The important quantity in the following is the sum of the derivatives of the phase shifts which we may conveniently express by $d/d\lambda\, Tr_0\, \Delta_\lambda$. The result to be established is given in

Theorem 3:

Let $R_z - \overset{0}{R}_z \in \mathscr{L}_1(\mathscr{H})$ (Trace class operators) for some (and hence for all) $z \in \varrho(H) \cap \varrho(\overset{0}{H})$, P be the projection on the subspace belonging to the point spectrum of H and let H and H_0 be bounded below.

Assume $\dim P < \infty$, then $\lim_{n\to\infty} Tr_0\, Q_\lambda^n$ exists in the sense of distributions and is given as follows, denoting the limit distributions as τ_λ,

$$\tau_\lambda = 2\frac{d}{d\lambda} Tr_0\, \Delta_\lambda + \sum_i n_i\, \delta_\lambda(\lambda_i)\,, \tag{21}$$

where Δ_λ is the 'phase shift' operator $\in \mathscr{L}_1(\mathscr{H}_0)$, (n_i, λ_i) are the multiplicity and eigenvalue respectively of H in the positive half-line.

Note that $R_z - \overset{0}{R}_z \in \mathscr{L}_1$ for one value of $z \in \varrho(H) \cap \varrho(\overset{0}{H})$ implies the same property for all values of z in the regularity domain. This was shown by Kato [5].

We defer the proof of Theorem 3 to Appendix B.

Formula (21) contains the final result of this paper. It establishes the relationship between the average time-delay represented by the quantity τ_λ on the left hand side and the phase shift of the scattering operator and the possible bound states appearing on the right.

This formula generalizes all previous results obtained before for the single channel case. It is also established under the weakest conditions known to us. Most applications are for the spherically symmetrical case and non-degenerate angular momentum states.

Appendix A

Proof of Theorem 1, Section 3

Let $\mathscr{G} = \int \oplus\, \mathscr{H}_\lambda\, d\lambda$ represent the direct integral of Hilbert space with respect to the absolutely continuous spectral family of $\overset{0}{H}$. It consists of equivalence classes of functions f_λ from $\Lambda \to \mathscr{H}_0$ a fixed Hilbert space $(\lambda \in \Lambda, f_\lambda \in \mathscr{H}_0)$. Two such functions are equivalent if they differ at most on a set of Lebesgue measure zero. They are square-integrable in the sense

$$\int \| f_\lambda \|_0^2 \, d\lambda < \infty$$

and we denote this integral as the *norm* of $\{f_\lambda\}$.

The set of such functions defines the Hilbert space $\mathscr{G}$. There exists then a one-to-one correspondance between the abstract Hilbert space $\mathscr{H}$ and the direct integral space which has in particular the property that if

$$f \leftrightarrow \{f_\lambda\} \quad \text{then} \quad \overset{0}{H} f \leftrightarrow \{\lambda f_\lambda\} \quad \text{and} \quad U_t f \leftrightarrow \{e^{-i\lambda t} f_\lambda\} .$$

This correspondance is an isomorphism in the sense that it preserves the entire Hilbert space structure, and in particular the norm:

$$\| f \|^2 = \int_\Lambda \| f_\lambda \|_0^2 \, d\lambda .$$

We define a dense linear subset $\mathscr{D} \subset \mathscr{G}$ by

$$\mathscr{D} = \{ f \in \mathscr{G} \mid \operatorname*{ess.sup}_{\lambda \in \Lambda} \| f_\lambda \|_0 < \infty \} .$$

Let $f \in \mathscr{D}$ and $\omega \in \mathscr{G}$ then we have

Lemma 1:

$$(f_\lambda, \omega_\lambda)_0 \in L^2(\Lambda) .$$

Proof: Schwartz' inequality in $\mathscr{H}_0$ gives

$$| (f_\lambda, \omega_\lambda)_0 |^2 \leq \| f_\lambda \|_0^2 \| \omega_\lambda \|_0^2 .$$

Hence

$$\int_\Lambda | (f_\lambda, \omega_\lambda)_0 |^2 \, d\lambda \leq \int_\Lambda \| f_\lambda \|_0^2 \|\omega_\lambda \|_0^2 \, d\lambda \leq \operatorname*{ess.sup}_{\lambda \in \Lambda} \| f_\lambda \|_0^2 \int \| \omega_\lambda \|_0^2 \, d\lambda$$

$$= \operatorname*{ess.sup}_{\lambda \in \Lambda} \| f_\lambda \|_0^2 \| \omega \|^2 .$$

Hence

$$(f_\lambda, \omega_\lambda)_0 \in L^2(\Lambda) .$$

Since

$$(f, U_t \omega) = \int_\Lambda e^{-i\lambda t} (f_\lambda, \omega_\lambda)_0 \, d\lambda$$

it follows from Parseval's relation and Lemma 1 that

$$\int_{-\infty}^{\infty} |(f, U_t\,\omega)|^2\,dt = 2\,\pi \int_{\Lambda} |(f_\lambda, \omega_\lambda)_0|^2\,d\lambda\,. \tag{A.1}$$

Lemma 2:

For all $f, g \in \mathscr{D}$ and $\Gamma \in \mathscr{L}_1$, the integral

$$G[f, g] \equiv \int_{-\infty}^{\infty} (f, U_t^*\,\Gamma\,U_t\,g)\,dt$$

converges absolutely.

Proof: Since Γ is trace class there exist two orthonormal families of vectors $u_r \in \mathscr{H}$, $v_r \in \mathscr{H}$ $(r = 1, 2, \ldots)$ and positive numbers $\alpha_1 \geq \alpha_2 \geq \cdots \geq 0$ such that

$$\Gamma = \sum_r \alpha_r\,v_r(u_r, .)\,.$$

This is the canonical representation of a compact operator. Since $\Gamma \in \mathscr{L}_1$, we have in addition

$$\sum_r \alpha_r = \|\Gamma\|_1 < \infty\,.$$

It follows that

$$\int_{-\infty}^{\infty} (f, U_t^*\,\Gamma\,U_t\,g)\,dt = \int_{-\infty}^{\infty} dt \sum_{r=1}^{\infty} \alpha_r(U_t f, v_r)\,(u_r, U_t\,g)\,.$$

The sequence of functions

$$f_n(t) = \sum_{r=1}^{n} \alpha_r(U_t f, v_r)\,(u_r, U_t\,g)$$

converges in the $L_t^1\,(-\infty, +\infty)$ norm since it is a Cauchy sequence in this norm and the space of L^1-functions is complete. This is due to the fact that

$$\int_{-\infty}^{\infty} |f_n(t) - f_m(t)|\,dt \quad (n > m)$$

$$= \int_{-\infty}^{\infty} \Big|\sum_{r=m}^{n} \alpha_r(U_t f, v_r)\,(u_r, U_t\,g)\Big|\,dt \leq \sum_{r=m}^{n} \alpha_r \int_{-\infty}^{\infty} |(U_t f, v_r)\,(u_r, U_t\,g)|\,dt$$

for $f \in \mathscr{D}$ and any v_r, $(U_t f, v_r) \in L_t^1(-\infty, +\infty)$ and for $g \in \mathscr{D}$ and any u_r, $(u_r, U_t\,g) \in L_t^1(-\infty, +\infty)$.

By using Schwartz' inequality we obtain

$$\sum_{r=m}^{n} \alpha_r \int_{-\infty}^{\infty} |\,(U_t f, v_r)\,(u_r, U_t g)\,|\,dt$$

$$\leq \sum_{r=m}^{n} \alpha_r \left(\int_{-\infty}^{\infty} |\,(U_t f, v_r)\,|^2\,dt\right)^{1/2} \left(\int_{-\infty}^{\infty} |\,(u_r, U_t g)\,|^2\,dt\right)^{1/2}$$

$$= (2\,\pi)^2 \sum_{r=m}^{n} \alpha_r \left(\int_{\Lambda} |(f_\lambda, v_{r\lambda})_0\,|^2\,d\lambda\right)^{1/2} \left(\int_{\Lambda} |\,(u_{r\lambda}, g_\lambda)_0\,|^2\,d\lambda\right)^{1/2}$$

$$\leq (2\,\pi)^2\,(\operatorname*{ess.sup.}_{\lambda\in\Lambda} \|\,f_\lambda\,\|_0^2)^{1/2}\,(\operatorname*{ess.sup.}_{\lambda\in\Lambda} \|\,g_\lambda\,\|_0^2)^{1/2} \sum_{r=m}^{n} \alpha_r \to 0$$

for $m, n \to \infty$.
This means

$$\lim_{n\to\infty} f_n(t) = \sum_{r=1}^{\infty} \alpha_r (U_t f, v_r)\,(u_r\, U_t\, g,) \in L_t^1(-\infty, \infty)$$

and this proves Lemma 2 and with it the first part of Theorem 1.

It follows then from known theorems on Lebesgue integration [4] that limits in the L^1-norm and integral can be interchanged, so that

$$G[f, g] = \sum_{r=1}^{\infty} \alpha_r \int_{-\infty}^{\infty} (U_t f, v_r)\,(u_r, U_t\, g)\,dt\,. \tag{A.2}$$

Using Parseval's theorem this becomes, after another interchange of limit and integral,

$$G[f, g] = 2\,\pi \int_{\Lambda} d\lambda \sum_{r=1}^{\infty} \alpha_r (f_\lambda, v_{r\lambda})_0\,(u_{r\lambda}, g_\lambda)_0\,. \tag{A.3}$$

If we define formally for a moment

$$G_\lambda \equiv 2\,\pi \sum_{r=1}^{\infty} \alpha_r\, v_{r\lambda} (u_{r\lambda}, \cdot)_0 \tag{A.4}$$

then we may write for the above expression

$$G[f, g] = \int_{\Lambda} d\lambda (f_\lambda, G_\lambda\, g_\lambda)_0\,.$$

In order to verify that the formal expression (A.4) represents a bounded operator we calculate

$$\|\,G_\lambda f_\lambda\,\|_0 \leq 2\,\pi \sum_{r=1}^{\infty} \alpha_r \,\|\,v_{r\lambda}\,\|_0\,|\,(u_{r\lambda}, f_\lambda)_0\,|$$

which, by Schwartz's inequality, can be majorized by

$$2\pi \sum_{r=1}^{\infty} \alpha_r \| v_{r\lambda} \|_0 \; \| u_{r\lambda} \|_0 \; \| f_\lambda \|_0 .$$

Since

$$\sum_r \alpha_r \int_\Lambda \| v_{r\lambda} \|_0 \; \| u_{r\lambda} \|_0 \, d\lambda \le \sum_r \alpha_r \left\{ \int_\Lambda \| v_{r\lambda} \|_0^2 \, d\lambda \right\}^{1/2} \left\{ \int_\Lambda \| u_{r\lambda} \|_0^2 \, d\lambda \right\}$$
$$= \sum_r \alpha_r < \infty$$

it follows that

$$2\pi \sum_{r=1}^{\infty} \alpha_r \| v_{r\lambda} \|_0 \; \| u_{r\lambda} \|_0$$

is finite almost everywhere and therefore G_λ is a bounded operator for almost all λ. This proves (14) of theorem 1.

Let us now estimate the trace norm of G_λ in $\mathscr{H}_0$. To this end we use the following definition of trace norm, viz.

$$\| G_\lambda \|_{01} \equiv \sup \sum_{s=1}^{\infty} | (\omega_s, G_\lambda \chi_s)_0 | ,$$

where the supremum is taken over all orthonormal systems of vectors $\{\omega_s\}$ and $\{\chi_s\}$ in $\mathscr{H}_0$.

Then

$$\| G_\lambda \|_{01} = 2\pi \sup \sum_{s=1}^{\infty} | \sum_{r=1}^{\infty} \alpha_r (\omega_s, v_{r\lambda})_0 \, (u_{r\lambda}, \chi_s)_0 | .$$

This double series converges absolutely since

$$\sum_r \alpha_r \sum_{s=1}^{\infty} | (\omega_s, v_{r\lambda})_0 \, (u_{r\lambda}, \chi_s)_0 | \le \sum_r \alpha_r \, (\sum_{s=1}^{\infty} | (\omega_s, v_{r\lambda})_0 |^2)^{1/2} \, (\sum_{s=1}^{\infty} | (u_{r\lambda}, \chi_s)_0 |^2)^{1/2}$$
$$= \sum_r \alpha_r \| v_{r\lambda} \|_0 \| u_{r\lambda} \|_0 < \infty \quad \text{for} \quad \text{a.a. } \lambda ,$$

as we have shown before and hence the trace norm is finite for a.a. λ.

We show next the G_λ are essentially unique in the sense that if G'_λ is another family, satisfying

$$G[f, g] = \int_\Lambda d\lambda (f_\lambda, G'_\lambda g_\lambda) \;\; \forall \; f, g \in \mathscr{D}$$

then $G_\lambda = G'_\lambda$ for a.a. $\lambda \in \Lambda$.

Indeed the above property would mean that for all functions $\varphi(\lambda)$ such that $\{\varphi(\lambda)\, g_\lambda\} \in \mathscr{D}$ we have

$$\int_\Lambda d\lambda\big(f_\lambda, (G_\lambda - G'_\lambda)\, g_\lambda\big)\, \varphi(\lambda) = 0 .$$

This condition is in particular satisfied for all bounded functions, and since they are a total set in $L^2(\Lambda)$, this implies

$$\big(f_\lambda, (G_\lambda - G'_\lambda)\, g_\lambda\big) = 0 \quad \text{a.e. in} \quad \Lambda .$$

As f, g run through $\mathscr{D}$ the components f_λ and g_λ run through the entire space $\mathscr{H}_0$ and thus

$$G_\lambda = G'_\lambda \quad \text{a.e. in} \quad \Lambda .$$

This proves that the operators G_λ are essentially unique.

Finally we verify the inequality (16). We obtain from (A.4) as before

$$\| G_\lambda \|_{01} \leq 2\,\pi \sum_{l=1}^{\infty} \alpha_l \, \| v_{l\lambda} \|_0 \, \| u_{l\lambda} \|_0 .$$

Integrating this over Λ and using Schwartz's inequality, we obtain

$$\begin{aligned}\int_\Lambda \| G_\lambda \|_{01}\, d\lambda &\leq 2\,\pi \sum_{l=1}^{\infty} \alpha_l \int_\Lambda \| v_{l\lambda} \|_0 \, \| u_{l\lambda} \|_0 \, d\lambda \\ &\leq 2\,\pi \sum_{l=1}^{\infty} \alpha_l \Big(\int_\Lambda \| v_{l\lambda} \|_0^2 \, d\lambda \Big)^{1/2} \Big(\int_\Lambda \| u_{l\lambda} \|_0^2 \, d\lambda \Big)^{1/2} \\ &= 2\,\pi \sum_{l=1}^{\infty} \alpha_l \\ &= 2\,\pi\, \| \Gamma \|_1 .\end{aligned}$$

This proves inequality (16) and the relation (15) can be similarly verified.

Appendix B

In this appendix, we shall first state without proof two theorems by Krein [6] and by Krein and Birman [7].

Theorem (Krein):

Let either (A) $H = \overset{0}{H} + V$ with $V \in \mathscr{L}_1(\mathscr{H})$, or (B) $R_z - \overset{0}{R}_z \in \mathscr{L}_1(\mathscr{H})$ for some $z \in \varrho(H) \cap \varrho(\overset{0}{H})$, then there exists a measurable function $\xi(\lambda)$ $(-\infty < \lambda < \infty)$ such that

$$T\,r(R_z - \overset{0}{R}_z) = -\int_{-\infty}^{\infty} \frac{\xi(\lambda)}{(\lambda - z)^2}\, d\lambda , \tag{B.1}$$

where $\xi(\lambda)$ has the following properties:

for condition (A): $\xi(\lambda) \in L^1(-\infty, \infty)$ and

$$\int_{-\infty}^{\infty} \xi(\lambda)\, d\lambda = Tr\, V$$

$$\text{and}\quad \xi(\lambda) = \frac{1}{\pi} \lim_{\epsilon \to 0^+} \operatorname{Im} \ln \det (1 + V \overset{0}{R}_{\lambda + i\epsilon}) \text{ a.e.}$$

and *for condition* (B): $\xi(\lambda)\ (1 + \lambda^2)^{-1} \in L^1(-\infty, \infty)$ and it is determined almost everywhere up to a constant. $\xi(\lambda)$ is called the spectral displacement function of $H, \overset{0}{H}$.

Theorem (Krein and Birman)

If the operators $H, \overset{0}{H}$ satisfy either condition (A) or (B), then the scattering matrix S_λ (the 'component' of the scattering operator S in $\mathscr{H}_\lambda$) is of the form:

$$S_\lambda = I_\lambda + T_\lambda \tag{B.2}$$

for almost all $\lambda \in \Lambda(\overset{0}{H})$, the spectrum of H_0, where I_λ is the identity operator and T_λ belongs in $\mathscr{L}_1(\mathscr{H}_\lambda)$. Furthermore, det $S_\lambda = e^{-2\pi i \xi(\lambda)}$ for almost all $\lambda \in \Lambda(\overset{0}{H})$ where $\xi(\lambda)$ is the function defined in the previous theorem.

Remark: From the representation

$$S_\lambda = I_\lambda + T_\lambda \quad \text{with} \quad T_\lambda \in \mathscr{L}_1(\mathscr{H}_\lambda)$$

we can conclude that there exists an operator $\Delta_\lambda \in \mathscr{L}_1(\mathscr{H}_\lambda)$ for a.a. $\lambda \in \Lambda(\overset{0}{H})$ such that $S_\lambda = e^{-2i\Delta_\lambda}$ for a.a. $\lambda \in \Lambda(\overset{0}{H})$. Furthermore, we can conclude that $Tr\, \Delta_\lambda = \pi\, \xi(\lambda)$ for a.a. $\lambda \in \Lambda(\overset{0}{H})$. A comparison with partial wave analysis in scattering theory justifies the name 'phase-shift' operator for Δ_λ.

We now prove the following proposition:

Proposition 1:

Assume that condition (A) of the above theorems is satisfied and let $\psi \in \mathscr{S}(\boldsymbol{R}^1)$, the class of C^∞ functions with rapid decrease at ∞, then $[\psi(H) - \psi(\overset{0}{H})] \in \mathscr{L}_1$ and

$$Tr\, [\psi(H) - \psi(\overset{0}{H})] = \int_{-\infty}^{\infty} \xi(\lambda)\, \psi'(\lambda)\, d\lambda\,. \tag{B.3}$$

The proof proceeds by a series of Lemmata.

Lemma 1: Let $A_n \in \mathscr{L}(\mathscr{H})$, $\| A_n \| \leq a$ and $A_n \to A$ strongly, let $B \in \mathscr{L}_1(\mathscr{H})$ (trace class), then

$$\lim_{n \to \infty} Tr\, A_n\, B = Tr\, A\, B\,. \tag{B.4}$$

Proof: Both $A_n\, B$ and $A\, B$ are trace class since A_n and A are bounded. Hence

$$Tr\, A_n\, B = \sum_{l=1}^{\infty} (\varphi_l\,, A_n\, B\, \varphi_l)$$

is independent of the orthonormal system $\{\varphi_l\}$. Let us choose for φ_l the eigenvectors of $B^*\, B$ so that

$$\sum_{l=1}^{\infty} \| B\, \varphi_l \| < \infty$$

then

$$|\, (\varphi_l\,, A_n\, B\, \varphi_l)\, | \leq \| A_n^*\, \varphi_l \|\, \| B\, \varphi_l \| \leq a\, \| B\, \varphi_l \|\,.$$

Hence the series $\sum_{l=1}^{\infty} (\varphi_l\,, A_n\, B\, \varphi_l)$ is absolutely convergent, uniformly in n and we can pass to the limit $n \to \infty$ term by term:

$$\begin{aligned}\lim_{n \to \infty} Tr\, A_n\, B &= \lim_{n \to \infty} \sum_{l=1}^{\infty} (\varphi_l\,, A_n\, B\, \varphi_l)\\ &= \sum_{l=1}^{\infty} \lim_{n \to \infty} (\varphi_l\,, A_n\, B\, \varphi_l) = \sum_{l=1}^{\infty} (\varphi_l\,, A\, B\, \varphi_l) = Tr\, A\, B\,.\end{aligned}$$

This proves Lemma 1.

Corollary: $A_n\, B \to A\, B$ in $\mathscr{L}_1$-norm topology.

Proof: Let $D_n = (A_n - A)^*\, (A_n - A) \in \mathscr{L}(\mathscr{H})$ and $\| D_n \| \leq c$, independent of n and $D_n \to 0$ strongly. Let $B = C\, D$ where $C, D \in \mathscr{L}_2(\mathscr{H})$.

Applying Lemma 1 to $T_r\, D_n\, C\, C^*$,

$$\begin{aligned}\| (A_n - A)\, C \|_2^2 &= Tr\, [\{(A_n - A)\, C\}^*\, (A_n - A)\, C]\\ &= Tr\, C^*\, D_n\, C = Tr\, D_n\, C\, C^* \underset{n \to \infty}{\to} 0\,.\end{aligned}$$

Hence

$$\begin{aligned}\| (A_n - A)\, B \|_1 &= \| (A_n - A)\, C\, D \|_1\\ &\leq \| (A_n - A)\, C \|_2\, \| D \|_2 \underset{n \to \infty}{\to} 0\,.\end{aligned}$$

Lemma 2: Let $R_z - \overset{0}{R}_z \in \mathscr{L}_1$, then

$$R_z^n - \overset{0}{R}{}_z^n \in \mathscr{L}_1 \quad (n = 1, 2 \ldots)$$

and

$$Tr\,(R_z^n - \overset{0}{R}{}_z^n) = -\,n \int_{-\infty}^{\infty} \frac{\xi(\lambda)}{(\lambda - z)^{n+1}}\, d\lambda\,. \tag{B.5}$$

Proof: That $R_z^n - \overset{0}{R}{}_z^n \in \mathscr{L}_1$ is trivial to see from the expression

$$R_z^n - \overset{0}{R}{}_z^n = R_z^{n-1}\,(R_z - \overset{0}{R}_z) + R_z^{n-2}\,(R_z - \overset{0}{R}_z)\,\overset{0}{R}_z + \cdots$$
$$\cdots + R_z\,(R_z - \overset{0}{R}_z)\,\overset{0}{R}{}_z^{n-2} + (R_z - \overset{0}{R}_z)\,\overset{0}{R}{}_z^{n-1}\,.$$

Since $d/dz\, R_z^{n-1} = (n-1)\, R_z^n$ exists in the norm-topology we find following Kato's holomorphy argument in page 547 of Ref. [5], that $R_z^{n-1} - \overset{0}{R}{}_z^{n-1}$ is holomorphic in the $\mathscr{L}_1$-norm and also

$$\frac{d}{dz}\,(R_z^{n-1} - \overset{0}{R}{}_z^{n-1}) = (n-1)\,(R_z^n - \overset{0}{R}{}_z^n)$$

in $\mathscr{L}_1$-norm sense.

We now proceed by induction. We assume that

$$R_z^{n-1} - \overset{0}{R}{}_z^{n-1} \in \mathscr{L}_1 \quad \text{and} \quad Tr\,(R_z^{n-1} - \overset{0}{R}{}_z^{n-1}) = -\,(n-1)\int \frac{\xi(\lambda)}{(\lambda - z)^n}\, d\lambda$$

we have

$$(n-1)\, Tr\,(R_z^n - \overset{0}{R}{}_z^n) = Tr\left[\frac{d}{dz}\,(R_z^{n-1} - \overset{0}{R}{}_z^{n-1})\right] = \frac{d}{dz}\, Tr\,(R_z^{n-1} - \overset{0}{R}{}_z^{n-1})$$
$$= \frac{d}{dz}\left\{-\,(n-1)\int \frac{\xi(\lambda)}{(\lambda - z)^n}\, d\lambda\right\} = -\,n(n-1)\int \frac{\xi(\lambda)}{(\lambda - z)^{n+1}}\, d\lambda\,.$$

We can differentiate inside the integral because the resulting integral is absolutely convergent. Therefore

$$Tr\,(R_z^n - \overset{0}{R}{}_z^n) = -\,n\int \frac{\xi(\lambda)}{(\lambda - z)^{n+1}}\, d\lambda \quad \text{for all} \quad z \in \varrho(H) \cap \varrho(\overset{0}{H})\,.$$

This proves Lemma 2.

Lemma 3: Let $V_n(t) \equiv \left(1 - \dfrac{i\,t\,H}{n}\right)^{-n}, \quad n = 1, 2, \ldots$

and $\overset{0}{V}_n(t) \equiv \left(1 - \dfrac{i\,t\,\overset{0}{H}}{n}\right)^{-n}, \quad n = 1, 2, \ldots,$

then $V_n(t) \underset{n\to\infty}{\to} e^{itH}$ strongly and similarly for $\overset{0}{V}_n(t)$. For the proof of this Lemma, the reader is referred to Kato [5], page 478–480.

Lemma 4: Let $\boldsymbol{\varphi}(t)$ be the Fourier transform of $\varphi(\lambda) \in \mathscr{S}(\boldsymbol{R}^1)$ and define $\varphi_n(H) \equiv \int_{-\infty}^{\infty} V_n(t)\, \boldsymbol{\varphi}(t)\, dt$, then $\varphi_n(H)$ is a bounded operator, defined everywhere and

$$\varphi_n(H) \underset{n\to\infty}{\overset{\text{weakly}}{\longrightarrow}} \varphi(H) \equiv \int_{-\infty}^{\infty} \varphi(\lambda)\, dE_\lambda .$$

Proof: That the integral is well-defined in Bochner-sense follows from the fact that $V_n(t)$ is strongly continuous for all t, $\| V_n(t) \| \leq 1$ and $\boldsymbol{\varphi} \in \mathscr{S}(\boldsymbol{R}^1)$.
Since

$$\int_{-\infty}^{\infty} \left(1 - \frac{i\,t\,\lambda}{n}\right)^{-n} \boldsymbol{\varphi}(t)\, dt \underset{n\to\infty}{\longrightarrow} \int_{-\infty}^{\infty} e^{it\lambda}\, \boldsymbol{\varphi}(t)\, dt = \varphi(\lambda)$$

and since

$$\int_{-\infty}^{\infty} d\, \| E_\lambda u \|^2 \int_{-\infty}^{\infty} \left| \left(1 - \frac{i\,t\,\lambda}{n}\right)^{-n} \boldsymbol{\varphi}(t) \right| dt < \infty$$

using Fubini's theorem and Lebesgue's dominated convergence theorem, we get the desired result.

Lemma 5: Let φ_n be as defined in the previous Lemma and assume condition (A), then $\varphi_n(H) - \varphi_n(\overset{0}{H}) \in \mathscr{L}_1(\mathscr{H})$ and it converges for $n \to \infty$ in trace-norm topology to $[\varphi(H) - \varphi(\overset{0}{H})]$.

Proof:

$$\varphi_n(H) - \varphi_n(\overset{0}{H}) = \int_{-\infty}^{\infty} [V_n(t) - \overset{0}{V}_n(t)]\, \boldsymbol{\varphi}(t)\, dt ,$$

$$V_n(t) - \overset{0}{V}_n(t) = 0 \quad \text{for} \quad t = 0$$

$$= \left(\frac{i\,n}{t}\right)^n (R^n_{-(in/t)} - \overset{0}{R}{}^n_{-(in/t)}) \quad \text{for} \quad t \neq 0 \quad \text{and hence}$$

$$V_n(t) - \overset{0}{V}_n(t) \in \mathscr{L}_1(\mathscr{H}) \quad \text{for all} \quad t \quad \text{and furthermore,}$$

$$\| V_n(t) - \overset{0}{V}_n(t) \|_1 \quad \text{for} \quad t \neq 0 ,$$

$$\leq \left| \frac{n}{t} \right|^n n \frac{1}{\left| \frac{n}{t} \right|^{n-1}} \| R_{-(in/t)} - \overset{0}{R}_{-(in/t)} \|_1 ,$$

$$\leq \left| \frac{n}{t} \right|^n n \frac{1}{\left| \frac{n}{t} \right|^{n-1}} \frac{1}{\left| \frac{n}{t} \right|^2} \| V \|_1 = | t | \; \| V \|_1 .$$

This shows that $V_n(t) - \overset{0}{V}_n(t)$ is continuous in $\mathscr{L}_1$-norm at $t = 0$ and since $\int_{-\infty}^{\infty} |t| \varphi(t)\, dt < \infty$, it follows that $\varphi_n(H) - \varphi_n(\overset{0}{H}) \in \mathscr{L}_1(\mathscr{H})$.

For showing the convergence, we take an auxiliary function $\psi(\lambda) \in \mathscr{S}(\boldsymbol{R}^1)$ defined as

$$\psi(\lambda) = \frac{\varphi(\lambda)}{1 + \lambda^2}\,.$$

Then

$$\psi(H) = \frac{1}{H^2 + 1}\, \varphi(H)$$

and

$$\psi(\overset{0}{H}) = \frac{1}{\overset{0}{H}{}^2 + 1}\, \varphi(\overset{0}{H})\,.$$

Let

$$\psi_n(H) = \frac{1}{H^2 + 1} \int_{-\infty}^{\infty} V_n(t)\, \varphi(t)\, dt\,.$$

From Kato [5], page 479, we obtain the following

$$\left[\frac{V_n(t) - V_m(t)}{H^2 + 1} - \frac{\overset{0}{V}_n(t) - \overset{0}{V}_m(t)}{\overset{0}{H}{}^2 + 1}\right] = \int_0^t ds \left(\frac{s}{n} - \frac{t-s}{m}\right)$$

$$\times \left\{\left(1 - \frac{i(t-s)}{m} H\right)^{-m-1} \left(1 - \frac{i\,s}{n} H\right)^{-n-1} \frac{H^2}{H^2 + 1}\right.$$

$$\left. - \left(1 - \frac{i(t-s)}{m} \overset{0}{H}\right)^{-m-1} \left(1 - \frac{i\,s}{n} \overset{0}{H}\right)^{-n-1} \frac{\overset{0}{H}{}^2}{\overset{0}{H}{}^2 + 1}\right\}.$$

That the integrand is actually trace class is trivial to see. Also it is easy to estimate it in $\mathscr{L}_1$-norm. It turns out that

$$\|\{\cdot\}\|_1 \le A + B\,s + C(t-s)\,; \quad A, B, C \text{ constants} \ge 0\,,$$

so that

$$\|\{[\psi_n(H) - \psi_n(\overset{0}{H})] - [\psi_m(H) - \psi_m(\overset{0}{H})]\}\|_1$$

$$\le \int_{-\infty}^{\infty} \left[\frac{A}{2}\left(\frac{1}{n} + \frac{1}{m}\right) t^2 + \left(\frac{B}{n} + \frac{C}{m}\right) \frac{|t|^3}{3} + \left(\frac{B}{m} + \frac{C}{n}\right) \frac{|t|^3}{6}\right] |\varphi(t)|\, dt$$

which shows the $\mathscr{L}_1$-convergence of $[\psi_n(H) - \psi_n(\overset{0}{H})]$ to

$$[\psi(H) - \psi(\overset{0}{H})] = \left[\frac{\varphi(H)}{H^2+1} - \frac{\varphi(\overset{0}{H})}{\overset{0}{H}{}^2+1}\right] \in \mathscr{L}_1 .$$

Proof of Proposition I:

Clearly

$$Tr\,[\psi(H) - \psi(\overset{0}{H})] = \lim_{n\to\infty} Tr\,[\psi_n(H) - \psi_n(\overset{0}{H})] .$$

Now,

$$Tr\left[\frac{V_n(t)}{H^2+1} - \frac{\overset{0}{V}_n(t)}{\overset{0}{H}{}^2+1}\right] \quad \text{for} \quad t \neq 0$$

$$= \left(\frac{i\,n}{t}\right)^n \frac{1}{(n-1)!}\left[\frac{d^{n-1}}{dz^{n-1}}\,Tr\left(\frac{R_z}{H^2+1} - \frac{\overset{0}{R}_z}{\overset{0}{H}{}^2+1}\right)\right]_{z=-(in/t)} \qquad \text{by Lemma 2.}$$

Using the resolvent equation and (B.1), the above reduces to

$$\left(\frac{i\,n}{t}\right)^n \frac{1}{(n-1)!}$$

$$\times\left[\frac{d^{n-1}}{dz^{n-1}}\left\{-\int_{-\infty}^{\infty}\frac{\xi(\lambda)}{(\lambda-z)^2\,(\lambda^2+1)}\,d\lambda - \int_{-\infty}^{\infty}\frac{2\,\lambda\,\xi(\lambda)}{(\lambda-z)\,(\lambda^2+1)^2}\,d\lambda\right\}\right]_{z=-(in/t)}$$

$$= \left(\frac{i\,n}{t}\right)^n (-1)$$

$$\times\left[n\int\frac{\xi(\lambda)}{(\lambda-z)^{n+1}\,(\lambda^2+1)}\,d\lambda + \int\frac{2\,\lambda\,\xi(\lambda)}{(\lambda-z)^n\,(\lambda^2+1)^2}\,d\lambda\right]_{z=-(in/t)} .$$

Differentiation in z inside the integral is allowed because the final integral is absolutely convergent.

Then

$$Tr\left[\frac{V_n(t)}{H^2+1} - \frac{\overset{0}{V}_n(t)}{\overset{0}{H}{}^2+1}\right]$$

$$= i\,t\int\frac{\xi(\lambda)}{\lambda^2+1}\left(1-\frac{i\,t\,\lambda}{n}\right)^{-n-1} d\lambda - \int\frac{2\,\lambda\,\xi(\lambda)}{(\lambda^2+1)^2}\left(1-\frac{i\,t\,\lambda}{n}\right)^{-n} d\lambda .$$

We note that this expression is actually valid also for $t = 0$.

Then

$$Tr\,[\psi_n(H) - \psi_n(\overset{0}{H})]$$

$$= \int_{-\infty}^{\infty} \varphi(t) \left\{ i\,t \int \frac{\xi(\lambda)}{\lambda^2+1} \left(1 - \frac{i\,t\,\lambda}{n}\right)^{-n-1} d\lambda - \int \frac{\xi(\lambda)\,2\,\lambda}{(\lambda^2+1)^2} \left(1 - \frac{i\,t\,\lambda}{n}\right)^{-n} d\lambda \right\} dt\,.$$

Since

$$\left| \left(1 - \frac{i\,t\,\lambda}{n}\right)^{-m} \right| \leq 1$$

and both $\int |\,\varphi(t)\,|\;|\,t\,|\,dt < \infty$, $\int |\,\varphi(t)\,|\,dt < \infty$ and also since

$$\int \frac{|\,\xi(\lambda)\,|}{\lambda^2+1}\,d\lambda < \infty$$

and

$$\left| \frac{2\,\lambda}{\lambda^2+1} \right| \leq 1\,,$$

applying Fubini's theorem, we obtain

$$Tr\,[\psi_n(H) - \psi_n(\overset{0}{H})]$$

$$= \int \frac{\xi(\lambda)}{\lambda^2+1}\,d\lambda \left\{ \int_{-\infty}^{\infty} \frac{i\,t\,\varphi(t)\,dt}{\left(1 - \frac{i\,t\,\lambda}{n}\right)^{n+1}} \right\} - \int \frac{\xi(\lambda)\,2\,\lambda}{(\lambda^2+1)^2}\,d\lambda \left\{ \int_{-\infty}^{\infty} \frac{\varphi(t)}{\left(1 - \frac{i\,t\,\lambda}{n}\right)^{n}}\,dt \right\}$$

and hence

$$Tr\,[\psi(H) - \psi(\overset{0}{H})]$$

$$= \int \frac{\xi(\lambda)}{\lambda^2+1} \left\{ \lim_{n\to\infty} \int \frac{i\,t\,\varphi(t)}{\left(1 - \frac{i\,t\,\lambda}{n}\right)^{n+1}}\,dt \right\} d\lambda$$

$$- \int \frac{\xi(\lambda)\,2\,\lambda}{(\lambda^2+1)^2} \left\{ \lim_{n\to\infty} \int \frac{\varphi(t)}{\left(1 - \frac{i\,t\,\lambda}{n}\right)^{n}}\,dt \right\} d\lambda\,.$$

That the limit $n \to \infty$ can be taken inside the integral is evident from the above argument. And now, we can again apply Lebesgue's dominated convergence theorem to the t-integrals to obtain

$$Tr\,[\psi(H) - \psi(\overset{0}{H})]$$

$$= \int \frac{\xi(\lambda)}{\lambda^2+1}\left\{\int_{-\infty}^{\infty} i\,t\,e^{it\lambda}\,\varphi(t)\,dt\right\}d\lambda$$

$$- \int \frac{\xi(\lambda)\,2\,\lambda}{(\lambda^2+1)^2}\left\{\int_{-\infty}^{\infty} e^{it\lambda}\,\varphi(t)\,dt\right\}d\lambda$$

$$= \int \xi(\lambda)\left[\frac{1}{\lambda^2+1}\,\frac{d\varphi(\lambda)}{d\lambda} - \frac{2\,\lambda}{(\lambda^2+1)^2}\,\varphi(\lambda)\right]d\lambda = \int \xi(\lambda)\,\psi'(\lambda)\,d\lambda\,.$$

Since every function ψ in $\mathscr{S}(\boldsymbol{R}^1)$ can be written in terms of another function φ in $\mathscr{S}(\boldsymbol{R}^1)$ such that $\psi(\lambda) = \varphi(\lambda)/1 + \lambda^2$ viz. choose $\varphi(\lambda) = (1+\lambda^2)\,\psi(\lambda)$, we have that

$$Tr\,[\psi(H) - \psi(\overset{0}{H})] = \int_{-\infty}^{\infty} \xi(\lambda)\,\psi'(\lambda)\,d\lambda \quad \text{for all} \quad \psi \in \mathscr{S}(\boldsymbol{R}^1)\,.$$

Lemma 6:

Let $S \in \mathscr{S}'$, the space of tempered distributions (see for example Ref. [8]) with support in the compact interval $[0, 1/b]$. Then one can find another distribution $T \in \mathscr{S}'$ (with support T in the half-line $[0, \infty]$) which is associated to S by the transformation:

$$\lambda' = \frac{1}{\lambda + b}\,, \quad \lambda \geq 0\,.$$

Proof: Let ψ be any function in $\mathscr{S}(\boldsymbol{R}^1)$. We define a C^∞-function $\hat{\varphi}$ as follows:

$$\hat{\varphi}(\lambda') = \lambda'^{-2}\,\psi\left(\frac{1 - b\,\lambda'}{\lambda'}\right) \quad \text{for} \quad \lambda' > 0$$

$$= 0 \qquad\qquad \text{for} \quad \lambda' \leq 0\,.$$

We also choose a C^∞-function ξ with following properties:

$$\xi(\lambda') = 1 \quad \text{for} \quad 0 \leq \lambda' \leq \frac{1}{b}$$

$$= 0 \quad \text{for either} \quad \lambda' \leq -\kappa_1$$

$$\text{or} \quad \lambda' \geq \frac{1}{b} + \kappa_2\,,$$

where κ_1, κ_2 are two positive numbers.

Denoting $\varphi(\lambda') = \xi(\lambda')\,\hat{\varphi}(\lambda')$, we observe that φ is a $\mathscr{D}$-function with support in $[-\kappa_1, (1/b) + \kappa_2]$. Now the definition of T to be associated with S is given by $(T, \psi) \equiv (S, \varphi)$.

From the above construction, it is clear that the above definition makes sense as a map $T\colon \mathscr{S} \to C$ and the map is linear. All we are then left to verify is the continuity of T. To do this, it suffices to show that if $\psi_n \to 0$ in $\mathscr{S}$-topology, $\varphi_n \to 0$ in $\mathscr{D}$-topology. We note that φ_n has support in $\mathscr{K} \equiv [-\kappa_1, (1/b) + \kappa_2]$ for all n.

$$\sup_{\lambda' \in \mathscr{K}} \left| \frac{d^p}{d\,\lambda'^p} \varphi_n(\lambda') \right|, \quad p \text{ any positive integer}$$

$$= \sup_{\lambda' \in \mathscr{K}} \left| \sum_{m=0}^{p} \binom{p}{m} \frac{d^m\,\xi(\lambda')}{d\lambda'^m} \frac{d^{p-m}}{d\lambda'^{p-m}} \hat{\varphi}_n(\lambda') \right|$$

$$\leq \sum_{m=0}^{p} \binom{p}{m} C_m(\xi) \sup_{\lambda} \left| \left((\lambda + b)^2 \frac{d}{d\lambda} \right)^{p-m} \{ (\lambda + b)^2\, \psi_n(\lambda) \} \right| .$$

In order to obtain the last inequality, we have used the fact that the functions $d^m\,\xi(\lambda')/(d\lambda'^m)$ (in $\mathscr{D}$) are bounded in the compact set $\mathscr{K}$ by, say, $C_m(\xi)$ and also we have used the transformation $\lambda' = 1/(\lambda + b)$. Since $\psi_n \to 0$ in $\mathscr{S}$-topology, the supremum in the last expression converges to zero as $n \to \infty$ and hence we have the required result.

To determine the support of the distribution T, one takes functions $\psi \in \mathscr{S}$ with support in the open set $\lambda < 0$. Then it follows from the construction of φ, that the corresponding φ has support in the open set $(1/b, (1/b) + \kappa_2)$ which is in the complement of the support of the distribution S. So clearly, support T is in closed right half-line, $[0, \infty]$.

Proof of Theorem 3:

Let $-b$ $(b > 0)$ be a real point in the common resolvent set of H and $\overset{0}{H}$ (which is possible because of the assumption on the spectra of H and $\overset{0}{H}$), then the operators $h_1 = \overset{0}{R}_{-b} = 1/(\overset{0}{H} + b)$ and $h_2 = R_{-b} = 1/(H + b)$ are self-adjoint bounded operators in $\mathscr{H}$ and also $v = h_2 - h_1 \in \mathscr{L}_1(\mathscr{H})$ (class of trace class operators).

Let $\varphi \in \mathscr{S}(\boldsymbol{R}^1)$. Proceeding in a similar fashion as in the derivation of equation (20), we conclude that

$$\int_0^\infty \frac{\tau_n(\lambda)\, \varphi\left(\dfrac{1}{\lambda + b}\right)}{(\lambda + b)^2}\, d\lambda = 2\,\pi\, Tr\, [\overset{0}{R}_{-b}\, T_{r_n}\, \overset{0}{R}_{-b}\, \varphi(h_1)]\,.$$

By a series of transformations, using the intertwining property of Ω, the commutativity of the trace, $\Omega^* \Omega = I - P$, and the resolvent identity, we obtain

$$\int_0^\infty \frac{\tau_n(\lambda)\, \varphi\left(\dfrac{1}{\lambda + b}\right)}{(\lambda + b)^2}\, d\lambda = 2\,\pi\, Tr\, \{ R_{-b}^2\, \varphi(h_2) - \overset{0}{R}{}_{-b}^2\, \varphi(h_1) \}\, P_{r_n}$$
$$- 2\,\pi\, Tr\, \{ R_{-b}^2\, \varphi(h_2)\, P \}\, P_{r_n}\,. \qquad \text{(B.6)}$$

In the above we have also used Proposition I, where $\psi(\lambda) = \lambda^2\,\varphi(\lambda)$, so that

$$\psi(h_2) - \psi(h_1) = R_{-b}^2\,\varphi(h_2) - \overset{0}{R_{-b}^2}\,\varphi(h_1) \in \mathscr{L}_1(\mathscr{H})\,.$$

We make the following transformation:

$$\lambda' = +\frac{1}{\lambda + b}\;(\lambda \geq 0)\,.$$

This maps the whole right half-line into the compact set $[0, 1/b]$. So far $\tau_n(\lambda)$ has been defined only for $\lambda \geq 0$, we extend this for $\lambda < 0$ by trivially defining $\tau_n(\lambda) = 0$ for $\lambda < 0$.

Identifying $\tau_n(\lambda) \equiv s_n(\lambda')$ for all $\lambda \geq 0$ or equivalently $\lambda' \in [0, +1/b]$, we can rewrite (B.6) as

$$\begin{aligned}\int_{1/b} s_n(\lambda')\,\varphi(\lambda')\,d\lambda' &= 2\,\pi\,T\,r\,\{h_2^2\,\varphi(h_2) - h_1^2\,\varphi(h_1)\}\,P_{r_n}\\ &\quad - 2\,\pi\,T\,r\,\{h_2^2\,\varphi(h_2)\,P\}\,P_{r_n}\,. \end{aligned}\tag{B.7}$$

Under the above change of variable, we can consistently define $s_n(\lambda') = 0$ for λ' outside $[0, 1/b]$, thereby obtaining

$$\begin{aligned}(s_n, \varphi) &\equiv \int_{-\infty}^{\infty} s_n(\lambda')\,\varphi(\lambda')\,d\lambda'\\ &= 2\,\pi\,Tr\,\{h_2^2\,\varphi(h_2) - h_1^2\,\varphi(h_1)\}\,P_{r_n} - 2\,\pi\,Tr\,\{h_2^2\,\varphi(h_2)\,P\}\,P_{r_n}\,.\end{aligned}\tag{B.8}$$

The left hand side makes sense because we had from equation (20) the fact that $\tau_n(\lambda)/(\lambda + b)^2 \in L^1[0, \infty]$ which implies $s_n(\lambda') \in L^1[-\infty, \infty]$. This leads us to conclude that $s_n \in \mathscr{S}'$, the space of tempered distributions.

Since $P_{r_n} \xrightarrow[n\to\infty]{\text{strongly}} 1$, we can use Lemma 1 to infer the existence of the limit (s_n, φ) as $n \to \infty$, for all $\varphi \in \mathscr{S}(\boldsymbol{R}^1)$. Let the limit distribution be denoted as s. Then by (B.3)

$$\begin{aligned}(s, \varphi) &= 2\,\pi\,T\,r\,[h_2^2\,\varphi(h_2) - h_1^2\,\varphi(h_1)] - 2\,\pi\,Tr\,h_2^2\,\varphi(h_2)\,P\\ &= 2\,\pi\int_{-\infty}^{\infty} \eta(\lambda')\,\frac{d}{d\lambda'}\left(\lambda'^2\,\varphi(\lambda')\right)d\lambda' - 2\,\pi\sum_{i\in\mathscr{I}} n_i\,\lambda_i'^2\,\varphi(\lambda_i')\,,\end{aligned}\tag{B.9}$$

where $\eta(\lambda')$ is the function in Krein's theorem corresponding to the system (h_2, h_1) and $\mathscr{I}$ is the finite family of indices denoting the eigenvectors of h_2, (n_i, λ_i') being their multiplicities and eigenvalues respectively.

(B.9) can be rewritten as a distribution equation as

$$s_{(\lambda')} = -\,2\,\pi\,\lambda'^2\,\frac{d}{d\lambda'}\,\eta(\lambda') - 2\,\pi\sum_{i\in\mathscr{I}} n_i\,\lambda_i'^2\,\delta(\lambda_i')\,,\tag{B.10}$$

δ being the Dirac-delta distribution and the derivative is taken in the sense of distribution. $s_{(\lambda')}$ has support in $[0, 1/b]$, since all $s_n(\lambda')$ has the same support.

From Krein's theorem (B.1) quoted in the beginning of this Appendix, we have

$$Tr\,[R_{z'}(h_2) - R_{z'}(h_1)] = -\int_{-\infty}^{\infty} \frac{\eta(\lambda')}{(\lambda' - z')^2}\, d\lambda' \quad (\operatorname{Im} z' \neq 0)$$

and

$$\eta(\lambda') = \frac{1}{\pi} \lim_{\epsilon \to 0^+} \operatorname{Im} \ln \det\,[1 + (h_2 - h_1)\, R_{\lambda' + i\epsilon}(h_1)]\,.$$

Let $H_0 \geq 0$ and $H \geq -\gamma > -b$, then $\operatorname{sp} h_1 = [0, 1/b]$ and $\operatorname{sp} h_2 \subset [0, 1/(b - \gamma)]$. So clearly $\eta(\lambda') = 0$ outside the domain $[0, 1/(b - \gamma)]$. Using the transformation $\lambda' = 1/(\lambda + b)$ and recalling the definitions of h_1 and h_2, the above integral representation reduces to

$$Tr\,(R_z - \overset{0}{R}_z) = -\int_{-\gamma}^{\infty} \frac{\eta\left(\dfrac{1}{\lambda + b}\right)}{(\lambda - z)^2}\, d\lambda\,, \quad \text{where} \quad z = \frac{1}{z'} - b\,,$$

and we can identify $\eta[1/(\lambda + b)] = \xi(\lambda)$ for $\lambda \geq -\gamma$.

In the region

$$\lambda \geq -\gamma > -b\,, \quad \lambda_i'^2\, \delta(\lambda_i') = \frac{1}{(\lambda_i + b)^2}\, \delta\left(\frac{1}{\lambda + b} - \frac{1}{\lambda_i + b}\right) = \delta(\lambda - \lambda_i)\,.$$

Since, by Lemma 6, we can associate a distribution $\tau_{(\lambda)} \in \mathscr{S}'$ with support in $[0, \infty]$ corresponding to $s_{(\lambda)'}$ with support in $[0, 1/b]$, we can write

$$\tau_{(\lambda)} = 2\pi \frac{d\xi(\lambda)}{d\lambda} + 2\pi \sum_{i \in \mathscr{I}} n_i\, \delta(\lambda_i)\,. \tag{B.10$'$}$$

Though the right hand side has support in $\lambda \geq -\gamma$ the distribution $\tau_{(\lambda)}$ has support in $\lambda \geq 0$ only. This implies that the restriction of the distribution

$$\left(\frac{d}{d\lambda}\, \xi(\lambda) + \sum_i n_i\, \delta(\lambda_i)\right) \quad \text{to} \quad -\gamma \leq \lambda < 0$$

is identically vanishing, thus allowing us to conclude that

$$\tau_{(\lambda)} = 2\pi \frac{d\xi(\lambda)}{d\lambda} + 2\pi \sum_{i \in \mathscr{I}^+} n_i\, \delta(\lambda_i)\,, \tag{B.11}$$

where $\mathscr{I}^+$ is the family of eigenvectors with positive eigenvalues of H.

Now we can use Krein-Birman's theorem as quoted before and arrive at the following:

$$\tau_{(\lambda)} = 2 \frac{d}{d\lambda}\, Tr_0\, \Delta_\lambda + 2\pi \sum_{i \in \mathscr{I}^+} n_i\, \delta(\lambda_i)\,, \tag{B.12}$$

where Δ_λ is the phase-shift operator explained before.

If there are no eigenstates with positive eigenvalues, then (B.11) reduces to Wigner's formula [9], viz.

$$\tau_\lambda = 2 \frac{d}{d\lambda} Tr_0 \Delta_\lambda . \tag{B.13}$$

It is also clear that if there are positive eigenvalues, then the particle is trapped in the scattering region and one expects the time-delay to be infinite. The precise sense in which the above equations hold, turns out to be in the sense of distributions.

Remark: If $V \in \mathscr{L}_1(\mathscr{H})$, then the above result can be proven much more easily. In fact it is a direct consequence of Proposition I. And in that case $\tau_n(\lambda)$'s converge directly in $\mathscr{S}'$-topology (weak) to a distribution $\tau_{(\lambda)}$. In the above case, viz., condition (B) with further assumption on the lower bound of H and H_0, it is easy to see that $\tau_n(\lambda)$'s in fact do not converge to $\tau_{(\lambda)}$ in $\mathscr{S}'$-topology, rather they converge in a topology, finer than $\mathscr{S}'$-topology.

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