Zeitschrift: Helvetica Physica Acta
Band: 44 (1971)
Heft: 3

Artikel: Stationary state scattering theory

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DOI: https://doi.org/10.5169/seals-114291

Stationary State Scattering Theory [1])

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Abstract. We give a rigorous mathematical derivation of the stationary state scattering theory from the time-dependent theory. The basic tool used is the spectral integral for operator valued functions with an operator valued measure. The chief result is the correct interpretation and validation of the formal expressions often used in stationary state scattering theory.

1. Introduction

There are two main approaches to the mathematical formulation of quantum mechanical scattering theory, the time-dependent and the time-independent or stationary state scattering theory. Most of the textbooks present both, but the precise relation between the two methods has remained elusive [6]. In this paper we shall establish the link between the two methods and thereby incidentally also justify some of the purely formal manipulations of the stationary method.

In the time-dependent scattering theory one considers the actual time-evolution of a wave packet for a particle under the influence of the interaction with a scattering center or with another particle. The asymptotic behavior of such wave packets in the remote past and the distant future is then approximately that of a free particle and the transition operator which connects the two asymptotic states is the scattering operator (or S-operator) which contains all the observable information on the scattering system.

In the stationary theory one studies solutions of the time-independent Schrödinger equation with an eigenvalue parameter belonging to the continuous part of the spectrum of the total Hamiltonian operator. These solutions lie outside the Hilbert space. They are characterized by certain asymptotic properties for large distances from the scattering center which are partly motivated by physical considerations. (For instance incident wave plus *outgoing* scattered wave.) The observable quantities, in particular the S-operator, are then obtained from the asymptotic properties of such solutions.

The two methods are mathematically very different, and it is not at all obvious that the final objects of the calculations, the S-operators, are indeed indentical for the two cases. It is therefore a natural question to ask whether the two methods are in fact equivalent.

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[1]) Based on a diploma thesis by V. Georgescu.

The question is difficult to answer because most presentations of stationary scattering theory use only formal mathematical manipulations which must first be interpreted in some sense before they can be made rigorous and then compared with the time-dependent method. The latter has become a well developed mathematical theory. An exposition and review of much of this work is found in Kato [15].

It is thus clear that, in order to carry out such a comparison and a study of the possible equivalence of the two methods, the stationary theory must first be developed on the same level of mathematical rigour as it has been possible for the time-dependent one.

This problem has been the object of much research during recent years. It does not have a unique solution. Indeed there have been at least four different methods used in order to complete the stationary scattering theory in the sense indicated above. A review of some of these methods will be found in the lectures of Kato and Kuroda [1].

In our opinion some of these methods, although completely correct from the mathematical point of view, use techniques which are sometimes rather removed from the conceptual context of the physicists. Thus for instance in the method of Kato and Kuroda one introduces a subset $X \subset \mathcal{H}$ of the Hilbert space, considered itself as a Banach space with its own independent norm, and one interprets some of the operators of the theory in this space. In the end result, after the construction of the wave and scattering operators has been accomplished, this space disappears. This fact and the fact that the choice of X is to some extent arbitrary may make this theory, in the view of a physicist, appear somewhat artificial, in spite of the fact that some very powerful results have been obtained with it.

Another technique which has been used is that of a generalized eigenfunction expansion for the total Hamiltonian operator. Here, too, some very important results were obtained but for their validity one needs assumptions for instance in the form of some gentleness or regularity conditions for the perturbation operator [16]–[18]. These assumptions, although certainly quite reasonable and very weak, have the disadvantage that they cannot easily be motivated in terms of the physical interpretation of the theory.

In view of these circumstances we have found it useful to develop further a method first proposed in connection with scattering theory by Galindo [14]. A similar approach was recently considered independently again by Prugovecki [3] and by Birman and Solomjak [4].

This method has the advantage that it does not need any other assumptions than the so-called strong asymptotic condition, which itself is directly interpretable in physical terms, together with the usual assumption concerning the range of the wave operators which is necessary for the unitarity of the scattering operator.

The essential mathematical tool used in this theory is a type of integral of an operator-valued function with an operator- (or vector-) valued measure which we shall call the *spectral integral*. Integrals of this kind have been used by mathematicians for some time [5]. Their usefulness for scattering theory is a relatively more recent discovery. Physicists have not yet used this kind of integration to any extent. We hope that through this paper they will become familiar with this mathematical tool and recognize it as the appropriate language for stationary scattering theory.

The spectral integral may be considered as a natural generalization of the functional calculus for operators, and its use permits us to formulate some of the important results in scattering theory with a certain conciseness and elegance. The manipulation of the integral is extremely easy and we shall show that several deeper lying results of scattering theory are readily obtainable with the help of this tool.

The principal problem that we propose to solve in this paper is the passage from the time-dependent to the stationary formalism. The basic quantities in the former theory (e.g. the wave operators) will first be expressed in terms of a Bochner integral of certain operators over the time variable. These integral formulas have been known for a long time and are indispensible in the mathematical development of time-dependent scattering theory. By the use of the functional calculus some of the operators in this Bochner integral will be expressed as a spectral integral. The two integrals can be interchanged and the time integral can then be evaluated. The remaining spectral integral is then the desired formula for the quantity in question. The main problem of mathematical nature is to establish under what conditions these two integrals can be interchanged and to verify that these conditions are in fact satisfied for the integrals that we encounter in scattering theory.

The organization of the paper is as follows: In Section 2 we introduce the two types of integrals used in this paper, the Bochner integral and the spectral integral. Section 3 gives the known results of the integral representations in the time-dependent formalism. Section 4 contains the main result in the form of theorem 3 which permits the passage from the Bochner integral to the spectral integral. In Section 5 we apply this result for the establishment of the principal basic formulae of the stationary state theory, and finally in Section 6 we give similar results for the scattering operator.

2. Mathematical Preliminaries

We shall need two types of integrals of operator valued functions, one with respect to a numerical valued measure on the reals and one with respect to a spectral measure for a selfadjoint operator. The former are called Bochner integrals, the latter spectral integrals.

The Bochner integral has been extensively treated in the literature. It suffices to give a brief summary of this integral here. For details we refer to the literature. In the applications that we have in view the functions to be integrated will always be continuous. We shall therefore give the definition of the Bochner integral for continuous functions in the form of a Riemann-Stieltjes integral. However, our main result (theorem 3) will be proved without continuity assumptions and makes use of the more general definition of Bochner integrability for arbitrary Borel functions [8].

Let $\mathcal{H}$ be a Hilbert space and f: $(a, b) \to \mathcal{H}$ a function from the finite interval (a, b) to vectors in $\mathcal{H}$, continuous in the strong (that is norm-) topology of $\mathcal{H}$. Let π: $a = \lambda_0 < \lambda_1 < \cdots < \lambda_n = b$ be a partition of (a, b), define $|\pi| = \sup_{i=1,\dots,n} |\lambda_i - \lambda_{i-1}|$

and choose for every i a point $\lambda_i' \in (\lambda_{i-1}, \lambda_i)$. We denote by $P(a, b)$ the set of all such partitions.

We define the Riemann sum

$$\Sigma_\pi(f) = \sum_{i=1}^{n} f(\lambda_i')\,(\lambda_i - \lambda_{i-1})\,. \tag{1}$$

If $\{\pi_r\}$ is a sequence of partitions from $P(a, b)$ such that $|\pi_r| \to 0$ for $r \to \infty$, the strong limit of $\Sigma_{\pi_r}(f)$ can be shown to exist and is called the Bochner integral of f with respect to the Lebesgue measure. We shall write

$$\int_a^b f(\lambda)\, d\lambda = s\text{-}\lim_{|\pi|\to 0} \Sigma_\pi(f) \tag{2}$$

and say that the function f is integrable (B).

If f: $\mathbf{R} \to \mathcal{H}$ is continuous and $\|f(\lambda)\|$ is Lebesgue integrable on (a, ∞), then

$$s\text{-}\lim_{b\to\infty} \int_a^b f(\lambda)\, d\lambda \tag{3}$$

exists and defines the Bochner integral of $f(\lambda)$ over the interval (a, ∞), and similarly for the lower limit $a \to -\infty$.

We have chosen the Riemann type integral and the strong limit. One can generalize the measure and use a weak definition of the Bochner integral. For the relation between the two see [9].

The fundamental theorem of Lebesgue is valid for Bochner integrals ([8], theorem 3.7.9). We shall use it in the following form:

Theorem (Lebesgue): Let (a, b) be a finite or infinite interval and f_n: $(a, b) \to \mathcal{H}$ a sequence of integrable functions (B) which converges almost everywhere to a function f: $(a, b) \to \mathcal{H}$. If there exists a Lebesgue integrable function g: $(a, b) \to \mathbf{R}$ such that almost everywhere $\|f_n(\lambda)\| \leqslant g(\lambda)$ for all n, then f is integrable (B) and

$$s\text{-}\lim_{n\to\infty} \int_a^b f_n(\lambda)\, d\lambda = \int_a^b f(\lambda)\, d\lambda\,. \tag{4}$$

This theorem gives thus the condition under which a limit can be interchanged with a Bochner-integral. It will be essential in the following.

The B-integral can easily be extended to functions whose values are bounded or even unbounded operators in $\mathcal{H}$. Indeed let u: $\lambda \to u(\lambda)$ $(\lambda \in (a, b) \subset \mathbf{R})$ be such a function and let $D_{u(\lambda)} \subseteq \mathcal{H}$ be the domain of the operator $u(\lambda)$. Let $\psi \in \mathcal{H}$ be such that $u(\lambda)\,\psi$ is defined for all $\lambda \in (a, b)$. If $\int_a^b u(\lambda)\,\psi\, d\lambda$ exists, we define

$$\left(\int_a^b u(\lambda)\, d\lambda\right)\psi = \int_a^b u(\lambda)\,\psi\, d\lambda \tag{5}$$

so that $\int_a^b u(\lambda)\, d\lambda$ is an operator defined on

$$\mathcal{D} = \left\{ \psi \in \mathcal{H} \mid \int_a^b u(\lambda) \, \psi \, d\lambda \text{ exists} \right\}. \tag{6}$$

Note that $\int_a^b u(\lambda) \, d\lambda$ may be unbounded even if all the operators $u(\lambda)$ are bounded. Furthermore the domain $\mathcal{D}$ may not be the largest domain on which the operator exists. In fact it may happen that the operator defined by (5) can be extended by continuity to a larger domain than $\mathcal{D}$. We shall presently see examples of this from scattering theory.

The foregoing theory of the B-integral can now be extended to the spectral integral in a formally analogous manner. To this end let us consider a spectral family E_λ, that is a non-decreasing family of projections as a function of $\lambda \in \mathbf{R}$. Let $\psi \in \mathcal{H}$ be fixed, $(a, b) \subset \mathbf{R}$ an arbitrary bounded interval and $u(\lambda)$ as above.

In complete analogy with (1) we define

$$\Sigma_\pi(u) = \sum_{i=1}^{n} u(\lambda_i') \left(E_{\lambda_i} - E_{\lambda_{i-1}} \right) \psi \, . \tag{7}$$

In order that this makes sense we require that

$$E_\lambda \, \psi \in \bigcap_{\mu \in (a,b)} D_{u(\mu)} \qquad \text{for all } \lambda \in (a, b) \, .$$

This is always the case if $D_{u(\lambda)} \supset D_H$ and $\psi \in D_H$ where $H = \int \lambda \, dE_\lambda$.

If the strong limit of $\Sigma_\pi(u)$ exists and is the same for all sequences of partitions $\pi \in P(a, b)$ such that $|\pi| \to 0$, then we define

$$\int_a^b u(\lambda) \, dE_\lambda \, \psi = s\text{-}\lim_{|\pi| \to 0} \Sigma_\pi(u) \, . \tag{8}$$

Just as before we can extend the definition to infinite intervals by taking strong limits. For instance for the interval (a, ∞) one defines

$$\int_a^\infty u(\lambda) \, dE_\lambda \, \psi = s\text{-}\lim_{b \to \infty} \int_a^b u(\lambda) \, dE_\lambda \, \psi \, . \tag{9}$$

A similar formula gives the integral for $(-\infty, a)$ and for $(-\infty, +\infty)$.

The integrals defined here are special cases of a more embracing integral theory which we shall not need here but only indicate briefly, in order to situate the theory in a more general mathematical context.

Let $\mathcal{X}, \mathcal{Y}, \mathcal{Z}$ be three Banach spaces and let there be given a continuous bilinear map from $\mathcal{X} \times \mathcal{Y}$ into $\mathcal{Z}$ such that

$$(x, y) \to x \, y = z \in \mathcal{Z} \, .$$

Let m: $\mathcal{B} \to \mathcal{Y}$ be a measure defined on the σ-algebra $\mathcal{B}$ of Borel subsets of a finite interval (a, b) of the real line. Let u: $(a, b) \to \mathcal{X}$ be a function on (a, b) with values in $\mathcal{X}$.

We are interested to define an integral of this function with respect to the measure m.

We define a partition π of (a, b) as a finite family of intervals $\Delta_i \in \mathcal{B}$ with the property

$$\Delta_i \cap \Delta_j = \emptyset \text{ if } i \neq j \text{ and } (a, b) = \bigcup_{i=1}^{n} \Delta_i .$$

Let μ be the Lebesgue measure on (a, b) and $|\pi| = \sup_i \mu(\Delta_i)$.

For every partition we form the generalized Riemann sum

$$\Sigma_\pi(u) = \sum_{i=1}^{n} u(\lambda_i') \, m(\Delta_i) \in \mathfrak{Z} \tag{10}$$

where $\lambda_i' \in \Delta_i$. Since $u(\lambda_i') \in \mathfrak{X}$, $m(\Delta_i) \in \mathfrak{Y}$, the sum of products of such terms is in $\mathfrak{Z}$ as indicated in formula (10). If the sum (10) converges for all sequences of partitions π such that $|\pi| \to 0$, then one defines the integral as the limit

$$\int_a^b u(\lambda) \, dm = \lim_{|\pi| \to 0} \Sigma_\pi(u) . \tag{11}$$

The limit is understood to be taken in the topology defined by the norm of the Banach space $\mathfrak{Z}$.

It is clear that the spectral integral defined by (8) is a special case of the integral (11) if the operators $u(\lambda)$ are bounded. To see this it suffices to identify

$$\mathfrak{X} = \mathfrak{B}(\mathcal{H}) , \quad \mathfrak{Y} = \mathcal{H} , \quad \mathfrak{Z} = \mathcal{H} ,$$
$$u\colon \mathsf{R} \to \mathfrak{B}(\mathcal{H}) , \quad m(\Delta) = E_\Delta \psi .$$

Integrals of the type (11) were studied by Bartle [11] and by Gowurin [12]. The theory is non-trivial in the sense that not every B-measurable and bounded function is integrable. An additional property of the measure is needed in order to ensure integrability of such functions [12]. In the special case which interests us we do not need the theory in its full generality so that the integrals in question always exist, as we shall demonstrate in the following.

For future reference we list five properties of the spectral integral that we shall frequently use in the rest of the paper.

(1) The operator valued function $u(\lambda)$ defined on the finite interval (a, b) is integrable with respect to the vector-valued measure $\lambda \mapsto E_\lambda \psi$ if and only if there exists a vector $\omega \in \mathcal{H}$ such that for every $\varepsilon > 0$ there exists a $\delta > 0$ with the property

$$\pi \in P(a, b) \text{ and } |\pi| < \delta \Rightarrow \|\omega - \Sigma_\pi(u)\| \leqslant \varepsilon .$$

(2) If u is integrable on (a, b) and on (b, c) (finite or infinite) with respect to $E_\lambda \psi$, then u is integrable on (a, c) and

$$\int_a^c u(\lambda) \, dE_\lambda \psi = \int_a^b u(\lambda) \, dE_\lambda \psi + \int_b^c u(\lambda) \, dE_\lambda \psi .$$

(3) If u_1, u_2 are integrable on (a, b) (finite or infinite) with respect to $E_\lambda \psi$ and if $B\colon \mathcal{H} \to \mathcal{H}$ is bounded, then $\lambda \mapsto B \, u_1(\lambda) + u_2(\lambda)$ is also integrable and

$$\int_a^b [B u_1(\lambda) + u_2(\lambda)] \, dE_\lambda \psi = B \int_a^b u_1(\lambda) \, dE_\lambda \psi + \int_a^b u_2(\lambda) \, dE_\lambda \psi .$$

(4) If u is integrable on (a, b) (finite or infinite) with respect to $E_\lambda \psi$, if A: $D_A \to \mathcal{H}$ $(D_A \subset \mathcal{H})$ is closed and if $A\, u(\lambda)$ is integrable on (a, b) with respect to $E_\lambda \psi$, then

$$A \int_a^b u(\lambda)\, dE_\lambda\, \psi = \int_a^b A\, u(\lambda)\, dE_\lambda \psi .$$

(5) If u is integrable on the interval (a, b) (finite or infinite) with respect to $E_\lambda \psi_1$ and $E_\lambda \psi_2$, then it is integrable on (a, b) with respect to $\lambda \mapsto E_\lambda (\alpha \psi_1 + \psi_2)$ $(\alpha \in \mathbf{C})$, and

$$\int_a^b u(\lambda)\, dE_\lambda (\alpha \psi_1 + \psi_2) = \alpha \int_a^b u(\lambda)\, dE_\lambda\, \psi_1 + \int_a^b u(\lambda)\, dE_\lambda \psi_2 .$$

Only property (1) is not immediately obvious, so we shall prove it here.

Proof of (1): Suppose first that u is integrable, and assume that the statement of (1) is not true. Then there exists an ε_0 such that for all $\delta > 0$ there exists a $\pi_\delta \in P(a, b)$ with $|\pi_\delta| < \delta$ and

$$\|\omega - \Sigma_{\pi_\delta}(u)\| > \varepsilon_0 .$$

Here we have written ω for the integral (which is supposed to exist). Choose $\delta_r = 1/r$, $r = 1, 2, \ldots$, then $\pi_r \equiv \pi_{\delta_r}$ satisfies $|\pi_r| \leqslant 1/r$ and $\|\omega - \Sigma_{\pi_r}(u)\| > \varepsilon_0$. Thus the sequence $\Sigma_{\pi_r}(u)$ does not converge to ω, which contradicts the hypothesis.

Conversely, suppose there exists a vector satisfying the conditions required in (1). Let π_r $(r = 1, 2, \ldots)$ be a sequence of partitions with $|\pi_r| \to 0$ for $r \to \infty$. It follows that $\|\omega - \Sigma_{\pi_r}(u)\| \to 0$ for $r \to \infty$. Since the sequence is arbitrary, the function $u(\lambda)$ is integrable.

This proves property (1) in full.

3. Integral Representations in the Time-Dependent Formalism

We shall assume in this section that we are dealing with a simple scattering system (for the definitions, cf. Jauch [13]). More specifically we impose the following conditions:

(θ) H_0 and $H = H_0 + V$ are selfadjoint on a common dense domain

$$\mathcal{D} \equiv D_H = D_{H_0} \tag{12}$$

and V is symmetric on a domain $D_V \supset \mathcal{D}$.

(A) For all $\psi \in \mathcal{H}$ the strong limits

$$s\text{-}\lim_{t \to \mp\infty} V_t^*\, U_t\, \psi = \psi_\pm \equiv \Omega_\pm \psi \tag{13}$$

exist where $V_t = e^{-iHt}$, $U_t = e^{-iH_0 t}$.

(B) H_0 has absolutely continuous spectrum.

(C) $R_+ = R_- = N$ where $R_\pm$ denotes the range of $\Omega_\pm$ and N is the orthogonal complement of the subspace spanned by the eigenvectors of H.

The conditions (A), (B) and (C) suffice for a complete theory of the time-dependent scattering formalism for simple systems.

The important quantities in this theory are

(1) the wave operators (Møller operators) $\Omega_{\pm}$,

(2) the scattering operator (Heisenberg operator) $S = \Omega_{-}^{*}\, \Omega_{+}$,

(3) $T_{\pm} = \Omega_{\pm} - I$,

(4) $R = S - I$,

The Møller operators have the interesting property

$$H\, \Omega = \Omega\, H_0 \tag{14}$$

and S as well as R commute with H_0

$$[R, H_0] = 0 = [S, H_0]\,. \tag{15}$$

The following theorem was proved in references [13, 14]:

Theorem 0:

(1) If (A) is satisfied, then

$$\Omega_{\pm} = s\text{-}\lim_{\varepsilon \downarrow 0} \Omega_{\pm\varepsilon}$$

where

$$\Omega_{+\varepsilon} = \varepsilon \int_{-\infty}^{0} e^{\varepsilon t}\, V_t^*\, U_t\, dt,$$

$$\Omega_{-\varepsilon} = \varepsilon \int_{0}^{\infty} e^{-\varepsilon t}\, V_t^*\, U_t\, dt\,.$$

(2) If (A), (B) and (C) are satisfied, then

$$\Omega_{\pm}^{*} = s\text{-}\lim_{\varepsilon \downarrow 0} \Omega_{\pm\varepsilon}^{*}$$

where

$$\Omega_{+\varepsilon}^{*} = \varepsilon \int_{-\infty}^{0} e^{\varepsilon t}\, U_t^*\, V_t\, dt\,,$$

$$\Omega_{-\varepsilon}^{*} = \varepsilon \int_{0}^{\infty} e^{-\varepsilon t}\, U_t^*\, V_t\, dt\,.$$

The integrals which are used here are integrals in the sense of Bochner, defined in Section 2. The proof is considerably simplified because the integrand consists of bounded operators only.

In the following we shall also use integral representations with unbounded integrands. In this case we need a further property which ensures sufficient regularity for the domains. This is exactly the property (θ).

Theorem 1:

(1) If (θ) and (A) are satisfied, then

$$\left.\begin{aligned} T_-|_{\mathcal{D}} &= s\text{-}\lim_{\varepsilon\downarrow 0} \; i\int_0^{\infty} e^{-\varepsilon t}\, V_t^*\, V\, U_t\, dt \\ T_+|_{\mathcal{D}} &= s\text{-}\lim_{\varepsilon\downarrow 0} - i\int_{-\infty}^{0} e^{\varepsilon t}\, V_t^*\, V\, U_t\, dt \end{aligned}\right\} \tag{16}$$

(2) If (θ), (A), (B) and (C) are satisfied, then in addition to the above representation (16), one has

$$\left.\begin{aligned} T_-^*|_{\mathcal{D}} &= s\text{-}\lim_{\varepsilon\downarrow 0} - i\int_0^{\infty} e^{-\varepsilon t}\, U_t^*\, V\, V_t\, dt \\ T_+^*|_{\mathcal{D}} &= s\text{-}\lim_{\varepsilon\downarrow 0} \; i\int_{-\infty}^{0} e^{\varepsilon t}\, U_t^*\, V\, V_t\, dt \end{aligned}\right\} \tag{17}$$

In the above formulae $T|_{\mathcal{D}}$ denotes the restriction of the operator T to the domain $\mathcal{D}$. Although $T = \Omega - I$ represents a bounded operator, the above equations are valid only on the common dense set $\mathcal{D}$.

Since the set $\mathcal{D}$ is dense, the operator T is the continuous extension to the entire Hilbert space of the operator $T|_{\mathcal{D}}$ as defined by the Bochner integrals of Theorem 1.

We precede the proof by establishing first

Lemma 1: Let A be a selfadjoint operator on a complex separable Hilbert space $\mathcal{H}$, $D_A \subset \mathcal{H}$ its domain of definition and $R_z = (A - z)^{-1}$ its resolvent operator ($z \in \mathbf{C} - \mathbf{R}$). If B is a linear operator with dense domain D_B and if

$$D_A \subset D_B\,, \quad D_A \subset D_{B^*}$$

then

(1) $B\,R_z$ is bounded for all $z \in \mathbf{C} - \mathbf{R}$,

(2) there exist two finite numbers $a, b \geqslant 0$ such that for all $\psi \in D_A$

$$\|B\,\psi\| \leqslant a\,\|A\,\psi\| + b\,\|\psi\|\,. \tag{18}$$

Proof: The operator $B\,R_z$ is defined everywhere, since $R_z(\mathcal{H}) \subset D_A \subset D_B$. If $\psi \in D_A \subset D_{B^*}$, then for all $\varphi \in \mathcal{H}$, we have by using the definition of an adjoint operator

$$(B\,R_z\,\varphi, \psi) = (R_z\,\varphi, B^*\,\psi) = (\varphi, R_z^*\,B^*\,\psi) = \big(\varphi, (B\,R_z)^*\,\psi\big)\,.$$

We write

$$(B\,R_z\,\varphi, \psi) = (\varphi, \psi^*) \;\text{ for all } \varphi \in \mathcal{H},\ \psi \in D_A\,.$$

We shall next verify that this relation is valid for all $\psi \in \mathcal{H}$. To see this, let $\psi \in \mathcal{H}$ and consider a sequence $\psi_n \in D_A$ such that $\psi = s\text{-}\lim_{n\to\infty} \psi_n$. Such a sequence exists, because D_A is dense in $\mathcal{H}$. For every $n = 1, 2, \ldots$, we have $(B\, R_z\, \varphi, \psi_n) = (\varphi, \psi_n^*)$. Since the left-hand side converges for $n \to \infty$ and for all $\varphi \in \mathcal{H}$, we have established that the sequence ψ_n^* converges weakly to a limit ψ^*, so that for this ψ^*

$$(B\, R_z\, \varphi, \psi) = (\varphi, \psi^*) \quad \text{for all } \varphi \in \mathcal{H}\,.$$

This shows that $\psi \in D_{(BR_z)^*}$. Since ψ was arbitrary in $\mathcal{H}$, it follows that $D_{(BR_z)^*} = \mathcal{H}$.

It follows then that $(B\, R_z)^*\, (B\, R_z)$ is symmetric and defined everywhere. Hence it is bounded. From this, it follows that $B\, R_z$ is also bounded, since for all $\psi \in \mathcal{H}$

$$\|B\, R_z\, \psi\|^2 = (B\, R_z\, \psi, B\, R_z\, \psi) = \big(\psi, (B\, R_z)^*\, B\, R_z\, \psi\big) \leqslant$$
$$\leqslant \|\psi\|\; \|(B\, R_z)^*\, B\, R_z\, \psi\| \leqslant \|(B\, R_z)^*\, B\, R_z\|\; \|\psi\|^2\,.$$

Furthermore, we have for all $\psi \in D_A$

$$\|B\, \psi\| = \|B\, R_i\, R_i^{-1}\, \psi\| \leqslant \|B\, R_i\|\; \|R_i^{-1}\, \psi\| \leqslant \|B\, R_i\|\, (\|A\, \psi\| + \|\psi\|)\,.$$

This finishes the proof of Lemma 1.

Lemma 2: If (θ) is satisfied and for $\psi \in \mathcal{D}$ we define

$$\psi_t = V_t^*\, U_t\, \psi\,, \quad \psi^t = U_t^*\, V_t\, \psi\,.$$

Then

$$\left.\begin{aligned} \frac{d\psi_t}{dt} &= i\, V_t^*\, V\, U_t\, \psi \\ \frac{d\psi^t}{dt} &= -i\, U_t^*\, V\, V_t\, \psi \end{aligned}\right\} \tag{19}$$

Furthermore the functions $t \mapsto V_t^*\, V\, U_t\, \psi$ and $t \mapsto U_t^*\, V\, V_t\, \psi$ are strongly continuous.

Proof of Lemma 2: We prove one half of the lemma, for instance that which refers to ψ_t, the other half is then almost identical. By Stone's theorem one has for any $\varphi \in \mathcal{D}$

$$\operatorname*{s-lim}_{\varepsilon \to 0} \left(\frac{V_{t+\varepsilon} - V_t}{\varepsilon} + i\, H\, V_t \right) \varphi = 0\,,$$

$$\operatorname*{s-lim}_{\varepsilon \to 0} \left(\frac{U_{t+\varepsilon} - U_t}{\varepsilon} + i\, H_0\, U_t \right) \varphi = 0\,.$$

Therefore

$$\frac{d\psi_t}{dt} = \operatorname*{s-lim}_{\varepsilon \to 0} \frac{1}{\varepsilon} (\psi_{t+\varepsilon} - \psi_t) = \operatorname*{s-lim}_{\varepsilon \to 0} \frac{1}{\varepsilon} (V_{t+\varepsilon}^*\, U_{t+\varepsilon} - V_t^*\, U_t)\, \psi$$

$$= \operatorname*{s-lim}_{\varepsilon \to 0} \left[\frac{1}{\varepsilon} (V_{t+\varepsilon}^*\, U_{t+\varepsilon} - V_{t+\varepsilon}^*\, U_t)\, \psi + \frac{1}{\varepsilon} (V_{t+\varepsilon}^*\, U_t - V_t^*\, U_t)\, \psi \right].$$

We decompose the first term on the right-hand side into two as follows

$$(V_{t+\varepsilon}^* - V_t^*)\, \frac{1}{\varepsilon} (U_{t+\varepsilon} - U_t)\, \psi + V_t^*\, \frac{1}{\varepsilon} (U_{t+\varepsilon} - U_t)\, \psi\,.$$

Here the second tends to $V_t^*(-i H_0)\, U_t\, \psi$ and the first tends to zero, because

$$\|(V_{t+\varepsilon}^* - V_t^*)\, \frac{1}{\varepsilon}\, (U_{t+\varepsilon} - U_t)\, \psi\| \leqslant$$

$$\leqslant \|(V_{t+\varepsilon}^* - V_t^*)\, (-i\, H_0\, \psi)\| + \|(V_{t+\varepsilon}^* - V_t^*)\left[\frac{1}{\varepsilon}\, (U_{t+\varepsilon} - U_t) + i\, H_0\right] \psi\|$$

and each term on the right tends separately to zero. Thus we find

$$\frac{d\psi_t}{dt} = V_t^*\, (-i\, H_0 + i\, H)\, U_t\, \psi = i\, V_t^*\, V\, U_t\, \psi$$

and this proves the first half of the statement of Lemma 2.

Let us verify next that the function $t \mapsto V_t^*\, V\, U_t\, \psi$ is strongly continuous for $\psi \in \mathcal{D}$. Since by assumption (θ), $D_{H_0} = \mathcal{D} \subset D_V \subset D_{V^*}$, we can use Lemma 1 to give for all $\psi \in \mathcal{D}$

$$\|V\, \psi\| \leqslant a\, \|H_0\, \psi\| + b\, \|\psi\| \quad (0 \leqslant a < \infty\,,\ 0 \leqslant b < \infty)\,.$$

Also, for any $\psi \in \mathcal{D}$

$$\|V_t^*\, V\, U_t\, \psi - V_{t_0}^*\, V\, U_{t_0}\, \psi\| \leqslant \|V_t^*\, V\, (U_t - U_{t_0})\, \psi\| + \|(V_t^* - V_{t_0}^*)\, V\, U_{t_0}\, \psi\|\,.$$

The second term obviously tends to zero since V_t is strongly continuous. The first term also tends to zero with $t_0 \to t$ because it is equal to

$$\|V\, (U_t - U_{t_0})\, \psi\| \leqslant a\, \|(U_t - U_{t_0})\, H_0\, \psi\| + b\, \|(U_t - U_{t_0})\, \psi\| \to 0\,.$$

This proves all of Lemma 2 referring to the functions ψ_t.

Now, we proceed to the proof of theorem 1.

Proof of Theorem 1: We prove the first of the relations (16). Let $\psi \in \mathcal{D}$ and $\varepsilon > 0$.

With lemma 2, we find that $d\psi_t/dt$ is strongly continuous. Thus for any finite interval $(a, b) \subset \mathbf{R}$ we can integrate the left-hand side of

$$\int_a^b e^{-\varepsilon t}\, \frac{d\psi_t}{dt}\, dt = i \int_a^b e^{-\varepsilon t}\, V_t^*\, V\, U_t\, \psi\, dt$$

by parts and obtain

$$\psi_b\, e^{-\varepsilon b} - \psi_a\, e^{-\varepsilon a} + \varepsilon \int_a^b e^{-\varepsilon t}\, \psi_t\, dt = i \int_a^b e^{-\varepsilon t}\, V_t^* V\, U_t\, \psi dt\ .$$

We set $a = 0$ and pass to the limit $b \to +\infty$. Finally we take the limit $\varepsilon \downarrow 0$ which exists because of condition (A) and theorem 0. Hence

$$T_-|_{\mathcal{D}} = s\text{-}\lim_{\varepsilon \downarrow 0}\, i \int_a^\infty e^{-\varepsilon t}\, V_t^*\, V\, U_t \psi\, dt\,.$$

This establishes the first of the relations (16). The proof for the other relations is similar and will be omitted.

Theorem 2:

If conditions (θ) and (A) are verified, then

$$\left.\begin{aligned} T_-|_{\mathcal{D}} &= \text{s-}\lim_{\varepsilon \downarrow 0} i \int_0^\infty e^{-\varepsilon t}\, U_t^*\, V\, \Omega_-\, U_t\, dt\,, \\ T_+|_{\mathcal{D}} &= \text{s-}\lim_{\varepsilon \downarrow 0} - i \int_{-\infty}^0 e^{\varepsilon t}\, U_t^*\, V\, \Omega_+\, U_t\, dt\,. \end{aligned}\right\} \tag{20}$$

Proof: Let $\psi \in \mathcal{D}$. The intertwining relation $H\,\Omega_- = \Omega_-\, H_0$ implies $\Omega_-(\mathcal{D}) \subset \mathcal{D}$. Thus $\Omega_-\,\psi \in \mathcal{D}$. Hence it follows from the second relation in (19) that

$$\frac{d(\Omega_-\,\psi)^t}{dt} = -\,i\, U_t^*\, V\, V_t\, \Omega_-\,\psi\,.$$

Reasoning in the same way as in the proof of theorem 1, we get

$$-\,\Omega_-\,\psi + \varepsilon \int_0^\infty e^{-\varepsilon t}\, U_t^*\, V_t\, \Omega_-\,\psi\, dt = -\,i \int_0^\infty e^{-\varepsilon t}\, U_t^*\, V\, V_t\, \Omega_-\,\psi\, dt\,.$$

Since $\Omega_-\,\psi \in R_-$, the strong limit as $\varepsilon \downarrow 0$ of the integral on the left-hand side exists as a consequence of assumption (A) and equals $\Omega_-^*\, \Omega_-\,\psi = \psi$. Using also $V_t\, \Omega_- = \Omega_-\, U_t$ for the right-hand member, we obtain

$$-\,(\Omega_- - I)\,\psi = \text{s-}\lim_{\varepsilon \downarrow 0} - i \int_0^\infty e^{-\varepsilon t}\, U_t^*\, V\, \Omega_-\, U_t\, \psi\, dt\,.$$

This proves the first of the relations (19). The second is proved similarly, and this establishes theorem 2.

The integral representations which are the content of theorems 1 and 2 have been known and used for a long time. We have established them here again in order to bring out the conditions and range for their validity, and to give a unified treatment in parallel with the spectral integral representations to be established in the next section.

Here we remark for the moment only that the formulae (16) and (20) have a certain kinship with the so-called *Lippmann–Schwinger* equations which one often finds in the literature on scattering theory as the basic equations for the stationary theory [6].

These equations are given in two forms

$$\text{‘}\psi_{in}^{(-)}(\lambda) = \psi_0(\lambda) - \frac{1}{H - \lambda + i\,\varepsilon}\, V\, \psi_0(\lambda)\text{’} \tag*{‘(16)’}$$

$$\text{‘}\psi_{in}^{(-)}(\lambda) = \psi_0(\lambda) - \frac{1}{H_0 - \lambda + i\,\varepsilon}\, V\, \psi_{in}^{(-)}(\lambda)\text{’}\,. \tag*{‘(20)’}$$

In these equations some sort of limit $\varepsilon \downarrow 0$ is to be taken. We have put them in quotes in order to emphasize their mathematically doubtful meaning and we have given them the equation numbers to which they correspond.

A similar pair of equations is obtained by reversing the sign of ε. They correspond to the second of the pair of equations (16) and (20).

From the integral representations (16) and (20), one obtains easily other integral representations for the S-operator which are also known but which we shall not need for the moment. We shall now rather concentrate on our main task of transcribing these integral representations into *spectral integrals* which furnish us the exact interpretation of equations such as '(16)' and '(20)'.

4. Spectral Integral Representations

In this section we shall derive the basic equations for the stationary state scattering theory. The procedure to be followed is the following:

In an integral such as the first of equation (16) we replace for instance the operator U_t by its spectral resolution $U_t = \int \exp(-i\lambda t)\, dE^0_\lambda$, where E^0_λ is the spectral family associated with the selfadjoint operator H_0, the generator of the group U_t. We obtain then a double integral, one over the spectral variable λ (the energy in the physical interpretation) and the other one over t (the time). If we interchange the order of integration, we observe that the resultant integral over t can be carried out to give a resolvent operator, and we arrive at the spectral integral representation of the operator Ω.

The important point in this sequence of manipulations is the interchange of the two integrals. If we were dealing with Lebesgue integration such an interchange could readily be justified by basing it on the fundamental theorem of Fubini. However our integrals are not of the Lebesgue type. There are three points of difference: the integrand is an operator-valued function, one of the measures is operator-valued and we have defined (for technical reasons) the integrals as Riemann-type integrals.

For these reasons the interchange of the two integrals needs a separate proof, which is the main content of this section. The proof is based on Lebesgue's theorem quoted at the beginning of Section 2 concerning the interchange of a limit with an integral.

Once this interchange of the integrals is established, we have a stationary state formalism which can be derived from the time-dependent one, and which has therefore the same degree of mathematical precision as the latter.

We begin this section with the crucial theorem which establishes the validity of the mentioned interchange of integrals.

Theorem 3:

Let

I. F_λ be a spectral family defining a selfadjoint operator $A = \int \lambda\, dF_\lambda$ in a separable Hilbert space $\mathcal{H}$,

II. (a, b) and (c, d) two (finite or infinite) intervals on the real line and $u: (a, b) \times (c, d) \to \mathbf{C}$ a complex valued function denoted by $u(\lambda, t)$, $\lambda \in (a, b)$ and $t \in (c, d)$,

III. B_t ($t \in \mathbf{R}$) a family of (not necessarily bounded) linear operators in $\mathcal{H}$,

IV. $\psi \in D_A$ a fixed vector in the domain of A.

Assume that:

(1) The integrals

$$\int_a^b u(\lambda, t)\, dF_\lambda \psi \quad \text{and} \int_a^b u(\lambda, t)\, dF_\lambda\, A\, \psi$$

exist for all $t \in (c, d)$.

(2) For all $t \in (c, d)$ one has $D_A \subset D_{B_t}$ and there exist positive constants α_t, β_t such that for every $\varphi \in D_A$

$$\|B_t \varphi\| \leqslant \alpha_t \|A\, \varphi\| + \beta_t \|\varphi\| .$$

(3) For all $\varphi \in D_A$ and for all $\lambda \in (a, b)$ the function $t \mapsto u(\lambda, t)\, B_t\, \varphi$ is integrable (B) on (c, d).

(4) There exists a function v: $(c, d) \to \mathbf{R}$ such that

(a) $|u(\lambda, t)| \leqslant v(t)$ for all $\lambda \in (a, b)$ and $t \in (c, d)$,

(b) $t \mapsto v(t)\, (\alpha_t \|A\, \psi\| + \beta_t \|\psi\|)$

is Lebesgue integrable on (c, d).

Then the existence of one of the two integrals

$$J = \int_c^d B_t \left(\int_a^b u(\lambda, t)\, dF_\lambda \psi \right) dt ,$$

$$J' = \int_a^b \left(\int_c^d u(\lambda, t)\; B_t\; dt \right) dF_\lambda\, \psi$$

entails the existence of the other one, and $J = J'$.

Proof: Suppose that J exists. We shall first establish that the operators B_t can be taken inside the spectral integral, i.e.

$$J = \int_c^d \left(\int_a^b u(\lambda, t)\; B_t\, dF_\lambda \psi \right) dt . \tag{21}$$

This is an immediate consequence of the assumptions (1) and (2) of the Theorem and of the following lemma:

Lemma 3: Let F_λ be the spectral family of the selfadjoint operator $A = \int \lambda\, dF_\lambda$, and let u: $\mathbf{R} \to \mathbf{C}$ be an integrable function on the (finite or infinite) interval $(a, b) \subset \mathbf{R}$ with respect to both of the measures $F_\lambda \psi$ and $F_\lambda\, A\, \psi$ for some $\psi \in D_A$. Suppose the linear operator B: $D_B \to \mathcal{H}$ $(D_B \subset \mathcal{H})$ satisfies the conditions $D_A \subset D_B$, and there exist $\alpha, \beta \geqslant 0$ such that for all $\psi \in D_A$

$$\|B\, \psi\| \leqslant \alpha \|A\, \psi\| + \beta \|\psi\| . \tag{22}$$

Then $\lambda \mapsto u(\lambda)\, B$ is integrable with respect to the measure $F_\lambda \psi$ and

$$B \int_a^b u\,(\lambda)\;\; dF_\lambda\;\; \psi = \int_a^b u(\lambda)\; B\, dF_\lambda \psi . \tag{23}$$

Proof of Lemma 3: Assume first that $(a, b) \subset \mathbf{R}$ is a finite interval. Let $\pi \in P(a, b)$ be a partition of (a, b) and write

$$\Sigma_\pi(u) = \sum_{i=1}^{n} u(\lambda_i') \, (F_{\lambda_i} - F_{\lambda_{i-1}}) \, \psi$$

for some $\psi \in D_A$. Evidently if $B\,u$ denotes the function $\lambda \mapsto u(\lambda)\, B$, we have

$$B\, \Sigma_\pi(u) = \sum_{i=1}^{n} u(\lambda_i') \, B\, (F_{\lambda_i} - F_{\lambda_{i-1}}) \, \psi = \Sigma_\pi(B\, u) \; .$$

To prove the lemma, we must show that (cf. Property (1) of section 2)

$$\Delta \equiv \| B \int_a^b u(\lambda)\, dF_\lambda \, \psi - \Sigma_\pi(B\, u) \| \to 0 \text{ with } |\pi| \to 0 \, .$$

According to the preceding remark this amounts to showing that

$$\| B \left[\int_a^b u(\lambda) \;\; dF_\lambda \; \psi - \Sigma_\pi(u) \right] \| \to 0 \quad \text{ with } |\pi| \to 0 \, .$$

If B were bounded the conclusion would follow trivially. For unbounded B we note that $\psi \in D_A$ and $\Sigma_\pi(u) \in D_A$. Next we verify that also $\int_a^b u(\lambda)\, dF_\lambda\, \psi \in D_A$. This follows from the fact that A is selfadjoint and hence closed. For $|\pi| \to 0$ both $\Sigma_\pi(u)$ and $A\, \Sigma_\pi(u) = \sum_{i=1}^{n} u(\lambda_i')\, (F_{\lambda_i} - F_{\lambda_{i-1}})\, A\, \psi$ converge by hypothesis. Hence $\int_a^b u(\lambda)\, dF_\lambda\, \psi \in D_A$ and

$$A \int_a^b u(\lambda)\, dF_\lambda\, \psi = \int_a^b u(\lambda)\, dF_\lambda\, A\, \psi \, . \tag{24}$$

It follows with (22) that

$$\Delta \leqslant \alpha \, \| A \left[\int_a^b u(\lambda)\, dF_\lambda \psi - \Sigma_\pi(u) \right] \| + \beta \, \| \int_a^b u(\lambda)\, dF_\lambda\, \psi - \Sigma_\pi(u) \| \, ,$$

and with $|\pi| \to 0$ both terms on the right tend to zero. Hence $s\text{-}\lim_{|\pi| \to 0} \Sigma_\pi(B\, u)$ exists and is equal to $B \int_a^b u(\lambda)\, dF_\lambda\, \psi$.

Suppose next that the interval (a, b) is infinite. It suffices to prove the case (a, ∞). Since u is integrable on (a, ∞) it is by definition integrable on any finite interval (a, b) with $a \leqslant b$, and

$$s\text{-}\lim_{b \to \infty} \int_a^b u(\lambda)\, dF_\lambda\, \psi = \int_a^\infty u(\lambda)\, dF_\lambda\, \psi \, .$$

For any finite b we have shown that

$$B \int_a^b u(\lambda)\, dF_\lambda\, \psi = \int_a^b u(\lambda)\, B\, dF_\lambda\, \psi \, .$$

Hence

$$\Delta_1 \equiv \| B \int_a^\infty u(\lambda)\, dF_\lambda \psi - \int_a^b u(\lambda)\, B dF_\lambda \psi \| =$$

$$= \| B \left[\int_a^\infty u(\lambda)\, dF_\lambda \psi - \int_a^b u(\lambda)\ dF_\lambda\ \psi \right] \| .$$

According to (24), one has for finite b

$$\int_a^b u(\lambda)\, dF_\lambda \psi \in D_A \quad \text{and} \quad A \int_a^b u(\lambda)\, dF_\lambda \psi = \int_a^b u(\lambda)\, dF_\lambda A\, \psi$$

and by hypothesis both expressions converge with $b \to \infty$. Since A is closed one can conclude

$$\int_a^\infty u(\lambda)\, dF_\lambda \psi \in D_A \quad \text{and} \quad A \int_a^\infty u(\lambda)\, dF_\lambda \psi = \int_a^\infty u(\lambda)\, dF_\lambda A\, \psi .$$

Hence, according to (22)

$$\Delta_1 \leqslant \alpha\ \| A \left[\int_a^\infty u(\lambda)\, dF_\lambda \psi - \int_a^b u(\lambda)\, dF_\lambda \psi \right] \| + \beta\ \| \int_a^\infty u(\lambda)\, dF_\lambda \psi - \int_a^b u(\lambda)\, dF_\lambda \psi \| .$$

Since both expressions on the right tend to zero with $b \to \infty$, one can conclude that $\Delta_1 \to 0$ with $b \to \infty$. This proves lemma 3.

We now continue with the proof of Theorem 3. Suppose first that (a, b) is finite, and let $\pi_N \in P(a, b)$ $(N = 1, 2, \ldots)$ be a sequence of partitions of the interval (a, b) with $|\pi_N| \to 0$ for $N \to \infty$. By definition

$$J = \int_c^d \left[s\text{-}\lim_{N \to \infty} f_N(t) \right] dt \tag{25}$$

with

$$f_N(t) = \sum_{i=1}^{n_N} u(\lambda_i'^N, t)\ B_t\ (F_{\lambda_i^N} - F_{\lambda_{i-1}^N})\ \psi .$$

By assumption (3) each $f_N(t)$ is integrable (B) on (c, d). Hence the proof of the theorem will be accomplished if we can prove the interchange of the (strong) limit $N \to \infty$ with the integral.

In order to do this, we apply the theorem of Lebesgue quoted at the beginning of Section 2. In order to show its applicability it suffices to show that the functions $f_N(t)$ are uniformly bounded by an integrable function on (c, d). For every N we have inequalities (we omit the index N on the right to simplify the notation)

$$\| f_N(t) \| = \| B_t \sum_{i=1}^{n} u(\lambda_i', t)\ (F_{\lambda_i} - F_{\lambda_{i-1}})\ \psi \|$$

$$\leqslant \alpha_t \, \| \sum_{i=1}^{n} u(\lambda'_i, t) \, (F_{\lambda_i} - F_{\lambda_{i-1}}) \, A \, \psi \| + \beta_t \, \| \sum_{i=1}^{n} u(\lambda'_i, t) \, (F_{\lambda_i} - F_{\lambda_{i-1}}) \, \psi \| \, . \tag{26}$$

Now, using condition (4a) of the hypotheses, we obtain for any $\varphi \in \mathcal{H}$

$$\| \sum_{i=1}^{n} u(\lambda'_i, t) \, (F_{\lambda_i} - F_{\lambda_{i-1}}) \, \varphi \|^2 = \sum_{i=1}^{n} | u(\lambda'_i, t) |^2 \, \| (F_{\lambda_i} - F_{\lambda_{i-1}}) \, \varphi \|^2 \leqslant$$

$$\leqslant v^2(t) \sum_{i=1}^{n} \| (F_{\lambda_i} - F_{\lambda_{i-1}}) \, \varphi \|^2 = v^2(t) \, \| \sum_{i=1}^{n} (F_{\lambda_i} - F_{\lambda_{i-1}}) \, \varphi \|^2 \leqslant$$

$$\leqslant v^2(t) \, \| \varphi \|^2 \, .$$

After substituting this inequality once with $\varphi = A \, \psi$ and once with $\varphi = \psi$ into (26), we obtain finally

$$\| f_N(t) \| \leqslant v(t) \, (\alpha_t \, \| A \, \psi \| + \beta_t \, \| \psi \|) \tag{27}$$

and this is integrable (L) by hypothesis (4b). This accomplishes the proof of theorem 3 for finite intervals (a, b).

Two more applications of Lebesgue's theorem permit us to extend the proof to infinite intervals. It suffices for instance to consider (a, ∞) with finite a.

Let b_N $(N = 1, 2, \ldots)$ be a sequence $a < b_N < \infty$, $b_N \to \infty$ with $N \to \infty$ and let

$$J_N = \int_c^d \left(\int_a^{b_N} u(\lambda, t) \, B_t \, dF_\lambda \, \psi \right) dt = \int_a^{b_N} \left(\int_c^d u(\lambda, t) \, B_t \, dt \right) dF_\lambda \, \psi \, .$$

The equality of the two expressions was just proved, since $b_N < \infty$. Thus it suffices to verify that

$$s\text{-}\lim_{N \to \infty} J_N = \int_c^d \left(\int_a^{\infty} u(\lambda, t) \, B_t \, dF_\lambda \, \psi \right) dt \, .$$

To see this, let

$$F_N(t) = \int_a^{b_N} u(\lambda, t) \, B_t \, dF_\lambda \, \psi$$

and let us verify first that $F_N(t)$ is integrable (B) on (c, d). Now

$$F_N(t) = s\text{-}\lim_{|\pi| \to 0} \sum_{i=1}^{n} u(\lambda'_i, t) \, B_t \, (F_{\lambda_i} - F_{\lambda_{i-1}}) \, \psi = s\text{-}\lim_{|\pi| \to 0} g_\pi^N(t) \, .$$

Each $g_\pi^N(t)$ is integrable (B) on (c, d), according to the hypothesis (3). Furthermore just as for (27) we have

$$\| g_\pi^N(t) \| \leqslant v(t) \, (\alpha_t \, \| A \, \psi \| + \beta_t \, \| \psi \|)$$

since this inequality is independent of the length of the interval (a, b_N). Applying the theorem of Lebesgue for the sequence $g_\pi^N(t)$ with fixed N and $|\pi| \to 0$, it follows that its limit $F_N(t)$ is also integrable (B). Furthermore

$$\| F_N(t) \| = \| B_t \int_a^{b_N} u(\lambda, t) \, dF_\lambda \, \psi \| \leqslant \alpha_t \, \| A \int_a^{b_N} u(\lambda, t) \, dF_\lambda \, \psi \| +$$

$$+ \beta_t \| \int_a^{b_N} u(\lambda, t)\, d F_\lambda \psi \| = \alpha_t \left[\int_a^{b_N} | u(\lambda, t) |^2 d \| F_\lambda A \psi \|^2 \right]^{1/2}$$

$$+ \beta_t \left[\int_a^{b_N} | u(\lambda, t) |^2 d \| F_\lambda \psi \|^2 \right]^{1/2} \leqslant v(t) (\alpha_t \|A \psi\| + \beta_t \|\psi\|)$$

and this is integrable (L) by hypothesis (4).

Thus Legesgue's theorem is again applicable for the sequence $F_N(t)$ with $N \to \infty$ and

$$J' = s\text{-}\lim_{N \to \infty} J_N = \int_c^d s\text{-}\lim_{N \to \infty} F_N(t)\, dt = J .$$

This proves one half of theorem 3. The proof of the other half is similar and will not be given here since it will not be needed in the following.

We shall also need a slightly different version of theorem 3 which can be proved in the same way as above:

Theorem 3':

Let the hypothesis of theorem 3 be true. Then the existence of one of the two integrals

$$K = \int_c^d dt \int_a^b u(\lambda, t)\, dF_\lambda B_t \psi ,$$

$$K' = \int_a^b dF_\lambda \int_c^d u(\lambda, t)\, B_t \psi\, dt$$

implies the existence of the other one and $K = K'$.

5. Applications of the Preceeding Results

As we have outlined at the beginning of the preceeding section the passage from time-dependent to the time-independent scattering theory is accomplished by the interchange of a Bochner integral with a spectral integral. The conditions for the validity of this operation were formulated in the hypotheses of theorem 3. It suffices now to verify that in scattering theory these conditions are verified and theorem 3 will supply us with a rich harvest of basic formulae in the stationary state formalism of scattering theory.

We denote by $R_z = (H - z)^{-1}$, $R_z^0 = (H_0 - z)^{-1}$ the two resolvent operators and we shall use the well known formulae

$$U_t = \int_{\mathbf{R}} e^{-i\lambda t}\, dE_\lambda^0 \qquad (28)_0$$

$$V_t = \int_{\mathbf{R}} e^{-i\lambda t}\, dE_\lambda , \qquad (28)$$

$$\left.\begin{aligned} R_z &= \quad i\int_0^\infty e^{izt}\, V_t\, dt \qquad Im\, z > 0 \\ R_z &= -i\int_{-\infty}^0 e^{izt}\, V_t\, dt \qquad Im\, z < 0 \end{aligned}\right\} \tag{29}$$

where E_λ^0 is the spectral family for H_0 and E_λ the spectral family for H.

Theorem 4:

If (A) is satisfied then

$$\Omega_- = \text{s-}\lim_{\varepsilon\downarrow 0} i\,\varepsilon\int_R R_{\lambda-i\varepsilon}\, dE_\lambda^0 = \text{s-}\lim_{\varepsilon\downarrow 0} -i\,\varepsilon\int_R dE_\lambda\, R_{\lambda+i\varepsilon}^0\,, \tag{30}$$

$$\Omega_+ = \text{s-}\lim_{\varepsilon\downarrow 0} -i\,\varepsilon\int_R R_{\lambda+i\varepsilon}\, dE_\lambda^0 = \text{s-}\lim_{\varepsilon\downarrow 0} i\,\varepsilon\int_R dE_\lambda\, R_{\lambda-i\varepsilon}^0\,. \tag{31}$$

If (A), (B) and (C) are satisfied, then

$$\Omega_-^* = \text{s-}\lim_{\varepsilon\downarrow 0} -\, i\,\varepsilon\int_R dE_\lambda^0\, R_{\lambda+i\varepsilon} = \text{s-}\lim_{\varepsilon\downarrow 0} i\,\varepsilon\int_R R_{\lambda-i\varepsilon}^0\, dE_\lambda\,, \tag{32}$$

$$\Omega_+^* = \text{s-}\lim_{\varepsilon\downarrow 0} i\,\varepsilon\int_R dE_\lambda^0\, R_{\lambda-i\varepsilon} = \text{s-}\lim_{\varepsilon\downarrow 0} -\, i\,\varepsilon\int R_{\lambda+i\varepsilon}^0\, dE_\lambda\,. \tag{33}$$

Proof: It suffices to prove a typical one of these formulae, for instance (30). By theorem 0 we have

$$\Omega_- = \text{s-}\lim_{\varepsilon\downarrow 0} \Omega_{-\varepsilon}$$

with

$$\Omega_{-\varepsilon}\psi = \varepsilon\int_0^\infty e^{-\varepsilon t}\, V_t^*\, U_t\,\psi\, dt = \varepsilon\int_0^\infty \left(V_t^* \int_R e^{-i(\lambda - i\varepsilon)t}\, dE_\lambda^0\,\psi\right) dt\,.$$

The hypotheses of theorem 3 are verified with $A = H_0$, $F_\lambda = E_\lambda^0$, $(a, b) = \mathsf{R}$, $(c, d) = (0, \infty)$, $u(\lambda, t) = \exp[-i\,(\lambda - i\,\varepsilon)\,t]$, $B_t = V_t^*$, $v(t) = \exp(-\varepsilon\, t)$, $\alpha_t = 0$, $\beta_t = 1$, and the theorem 3 gives

$$\Omega_{-\varepsilon}\,\psi = i\,\varepsilon\int_R R_{\lambda-i\varepsilon}\, dE_\lambda^0\,\psi\,.$$

Passing to the limit $\varepsilon \to +0$ gives (30). The proof of the first part of the other formulae is similar and can be omitted. The second equalities in (30)–(33) can be obtained in the same way by using theorem 3′.

Theorem 5:

Suppose that conditions (θ) and (A) are satisfied. Then

$$T_-|_{\mathcal{D}} = \text{s-}\lim_{\varepsilon\downarrow 0} -\int_R R_{\lambda-i\varepsilon}\, V\, dE_\lambda^0 = \text{s-}\lim_{\varepsilon\downarrow 0}\int_R dE_\lambda\, V\, R_{\lambda+i\varepsilon}^0\,, \tag{34}$$

$$T_+ \big|_{\mathcal{D}} = s\text{-}\lim_{\varepsilon \downarrow 0} - \int_{\mathbf{R}} R_{\lambda+i\varepsilon}\, V\, dE_\lambda^0 = s\text{-}\lim_{\varepsilon \downarrow 0} \int_{\mathbf{R}} dE_\lambda\, V\, R^0_{\lambda-i\varepsilon}\,. \tag{35}$$

Suppose that conditions (θ), (A), (B) and (C) are verified. Then

$$T_-^* \big|_{\mathcal{D}} = s\text{-}\lim_{\varepsilon \downarrow 0} - \int_{\mathbf{R}} dE_\lambda^0\, V\, R_{\lambda+i\varepsilon} = s\text{-}\lim_{\varepsilon \downarrow 0} \int_{\mathbf{R}} R^0_{\lambda-i\varepsilon}\, V\, dE_\lambda\,, \tag{36}$$

$$T_+^* \big|_{\mathcal{D}} = s\text{-}\lim_{\varepsilon \downarrow 0} - \int_{\mathbf{R}} dE_\lambda^0\, V\, R_{\lambda-i\varepsilon} = s\text{-}\lim_{\varepsilon \downarrow 0} \int_{\mathbf{R}} R^0_{\lambda+i\varepsilon}\, V\, dE_\lambda\,. \tag{37}$$

Proof: It suffices to prove a typical one of these formulae, for instance (34). We start with the first of equation (16), and choose a $\psi \in \mathcal{D}$.

$$T_{-\varepsilon}\, \psi = i \int_0^\infty e^{-\varepsilon t}\, V_t^*\, V\, U_t\, \psi\, dt = i \int_0^\infty dt\, V_t^*\, V \int_{\mathbf{R}} e^{-i(\lambda - i\varepsilon)t}\, dE_\lambda^0\, \psi\,.$$

In theorem 3 we now choose $A = H_0$, $F_\lambda = E_\lambda^0$, $(a, b) = \mathbf{R}$, $(c, d) = (0, \infty)$, $u(\lambda, t) = \exp[-i\, (\lambda - i\, \varepsilon)\, t]$, $B_t = V_t^*\, V$. Condition 1 is then satisfied. For condition 2 we remark that according to (θ) and Lemma 1

$$\|V_t^*\, V\, \psi\| = \|V\, \psi\| \leqslant \alpha\, \|H_0\, \psi\| + \beta\, \|\psi\|\,.$$

Thus for condition 2 it suffices to choose $\alpha_t = \alpha$, $\beta_t = \beta$. Condition 3 is satisfied because $t \mapsto \exp[-i\, (\lambda - i\, \varepsilon)\, t]\, V_t^*\, V\, \varphi$ is strongly continuous and bounded by $\exp(-\varepsilon\, t)\, \|V\, \varphi\|$. For condition (4) we put $v(t) = \exp(-\varepsilon\, t)$.

Thus theorem 3 applies and we can exchange the integration to obtain the first part of (34).

For the second part of (34) we must reason differently. Here we have to take $A = H$, $F_\lambda = E_\lambda$, $B_t = V\, U_t$. From (θ) and Lemma 1 we know also that there exist $\alpha, \beta \geqslant 0$ such that

$$\|V\, \psi\| \leqslant \alpha\, \|H\, \psi\| + \beta\, \|\psi\| \quad \text{for all } \psi \in \mathcal{D}\,.$$

Thus

$$\psi \in \mathcal{D} \Rightarrow U_t\, \psi \in \mathcal{D} \Rightarrow \|V\, U_t\, \psi\| \leqslant \alpha\, \|H\, U_t\, \psi\| + \beta\, \|\psi\|\,.$$

Using twice again Lemma 1, we have for $\varphi \in \mathcal{D}$

$$\|H\, \varphi\| \leqslant \alpha'\, \|H_0\, \varphi\| + \beta'\, \|\varphi\| \qquad (\alpha', \beta' \geqslant 0)$$

and

$$\|H_0\, \varphi\| \leqslant \alpha''\, \|H\, \varphi\| + \beta''\, \|\varphi\| \qquad (\alpha'', \beta'' \geqslant 0)$$

so that

$$\|V\, U_t\, \psi\| \leqslant \alpha\, \alpha'\, \|H_0\, \psi\| + \alpha\, \beta'\, \|\psi\| + \beta\, \|\psi\| \leqslant$$
$$\leqslant \alpha\, \alpha'\, \alpha''\, \|H\, \psi\| + [\alpha\, \alpha'\, \beta'' + \alpha\, \beta' + \beta]\, \|\psi\|\,.$$

Condition 2 of theorem 3 is then satisfied with

$$\alpha_t = \alpha\, \alpha'\, \alpha''\,, \qquad \beta_t = \alpha\, \alpha'\, \beta'' + \alpha\, \beta' + \beta\,.$$

For condition 3 we note that $t \mapsto V\, U_t\, \psi$ is strongly continuous (cf. the last inequality in the proof of Lemma 3) and $\|V\, U_t\, \psi\| \leqslant \alpha'''\, \|H_0\, \psi\| + \beta'''\, \|\psi\|$. Conditions (1) and (4) are then also satisfied and the second part of (34) follows from theorem 3′.

Theorem 6:

If (θ) and (A) are satisfied then

$$T_-|_{\mathcal{D}} = s\text{-}\lim_{\varepsilon \downarrow 0} - \int_R R^0_{\lambda - i\varepsilon} V \Omega_- dE^0_\lambda = s\text{-}\lim_{\varepsilon \downarrow 0} \int_R dE^0_\lambda V \Omega_- R^0_{\lambda + i\varepsilon} , \tag{38}$$

$$T_+|_{\mathcal{D}} = s\text{-}\lim_{\varepsilon \downarrow 0} - \int_R R^0_{\lambda + i\varepsilon} V \Omega_+ dE^0_\lambda = s\text{-}\lim_{\varepsilon \downarrow 0} \int_R dE^0_\lambda V \Omega_+ R^0_{\lambda - i\varepsilon} . \tag{39}$$

Proof: One starts with formulae (20) and uses the same procedure as for the proof of theorem 5. This accomplishes the proof of theorem 6.

The formulae of the last three theorems constitute the 'Lippmann-Schwinger' equations of the stationary scattering theory. In particular the merely formal equations '(16)' and '(20)' correspond to (34) and (38) respectively.

Once this correspondence is established one can proceed step by step to transform the 'derivations' of the formal theory into correct equations. We shall illustrate this procedure by deriving some standard results for the S- and R-operator ($R = S - I$) in the stationary state theory.

6. The Scattering Operator in the Stationary State Theory

We shall now derive certain expressions for the R-operator, where $R = S - I$ and $S = \Omega^*_- \Omega_+$ is the scattering operator.

Since both S and R commute with H_0, they are operators on the energy shell only. They can be expressed in terms of the operators $V \Omega_+$ and $\Omega^*_- V$ for instance, by omitting from them all the matrix elements belonging to different values of the energy. The resulting two operators on the energy shell are then equal and coincide with the R-operator up to a factor $-2\pi i$.

This procedure of reducing a given operator to the energy shell is not easy to formulate correctly since one must somehow produce a δ-function with respect to the energy variable and such a δ-function has only meaning as a distribution operating on a test function space. In many applications, there is no assurance that the matrix elements are functions from a test function space (unless one specifically postulates this) and then the formal manipulations can be made rigorous only under very specific and unphysical hypotheses.

All this is not needed in the spectral integral representation and it is just precisely at this point where the elegance and power of this technique are most evident.

The δ-function is in this formalism replaced by the 'pinch'-operator $\Pi_\lambda \equiv R^0_{\lambda - i\varepsilon} - R^0_{\lambda + i\varepsilon}$ which is diagonal in the spectral representation of H_0 with the following diagonal matrix element

$$\Pi_\lambda(\mu) = - \frac{2 i \varepsilon}{(\mu - \lambda)^2 + \varepsilon^2} \, .$$

It is well-known that for $\varepsilon \downarrow 0$ this tends to $-2\pi i \delta(\mu - \lambda)$. In the spectral integral form we need not use a representation for the operators in question and the limit is valid in the strong operator topology (and not as a point-wise limit).

More precisely this is formulated in the following

Theorem 7:

If the conditions (θ) and (A) are satisfied, then

$$R\big|_{\mathcal{D}} = \operatorname*{s-lim}_{\varepsilon\downarrow 0}\int_{R} (R^0_{\lambda-i\varepsilon} - R^0_{\lambda+i\varepsilon})\, \Omega_-^*\, V\, dE^0_\lambda = \operatorname*{s-lim}_{\varepsilon\downarrow 0}\int_{R} dE^0_\lambda\, \Omega_-^*\, V\, (R^0_{\lambda-i\varepsilon} - R^0_{\lambda+i\varepsilon})\,. \tag{40}$$

If the conditions (θ), (A), (B) and (C) are satisfied then

$$R\big|_{\mathcal{D}} = \operatorname*{s-lim}_{\varepsilon\downarrow 0}\int_{R} (R^0_{\lambda-i\varepsilon} - R^0_{\lambda+i\varepsilon})\, V\, \Omega_+\, dE^0_\lambda = \operatorname*{s-lim}_{\varepsilon\downarrow 0}\int_{R} dE^0_\lambda\, V\, \Omega_+\, (R^0_{\lambda-i\varepsilon} - R^0_{\lambda+i\varepsilon})\,. \tag{41}$$

Proof: From the definition $S = \Omega_-^*\, \Omega_+$ it follows that

$$R = S - I = \Omega_-^*\,(\Omega_+ - \Omega_-) = \Omega_-^*\,(T_+ - T_-)\,.$$

Using the first part of (34) and (35) we find for $\psi \in \mathcal{D}$

$$R\,\psi = \Omega_-^*\, \operatorname*{s-lim}_{\varepsilon\downarrow 0}\int_{R} (R_{\lambda-i\varepsilon} - R_{\lambda+i\varepsilon})\, V\, dE^0_\lambda\, \psi\,.$$

Since Ω_-^* is bounded, we can take it inside the limit and the integral. After using the intertwining relation in the form $\Omega_-^*\, R_z = R^0_z\, \Omega_-^*$ we obtain the desired result, the first part of formula (40):

$$R\big|_{\mathcal{D}} = \operatorname*{s-lim}_{\varepsilon\downarrow 0}\int_{R} (R^0_{\lambda-i\varepsilon} - R^0_{\lambda+i\varepsilon})\, \Omega_-^*\, V\, dE^0_\lambda\,.$$

For the second formula (41) we use

$$R = (\Omega_-^* - \Omega_+^*)\,\Omega_+ = (T_-^* - T_+^*)\,\Omega_+$$

and substitute the second part of the expressions (36) and (37). Taking account of the intertwining relation $E_\lambda\, \Omega_+ = \Omega_+\, E^0_\lambda$ we arrive at the first part of the formula (41). The proof for the second half of (40) and (41) is similar and need not be given here. This proves theorem 7.

The equations (40) and (41) express the R-operator in terms of the potential V and of the wave operators $\Omega_\pm$. They correspond to formula (7.40) in reference [6]. Our final result will be the establishment of a formula for the R-operator in terms of the resolvent $R_{\lambda+i0}$ and the interaction operator. This is the formula (7.41) in reference [6]. It may be loosely stated as

$$\text{`}R(\lambda) = -2\pi i\,(V - V\,R_{\lambda+i0}\,V)\text{'} \qquad \text{`(42)'}$$

where $R(\lambda)$ is the operator $S - I$ on the energy shell (not to be confused with the resolvent operator $R_{\lambda+i0}$!)

It may be obtained from the first of equation (41) by replacing Ω_+ by its own spectral integral representation, for instance from the first of equation (35).

This procedure involves two problems of mathematical nature, the first concerns the reduction of a double spectral integral to a single integral and the second the exact meaning and validity of a double limit $\varepsilon \downarrow 0$.

If we carry out the above-mentioned substitution of (35) into (41) we obtain for all $\psi \in \mathcal{D}$

$$R\,\psi = s\text{-}\lim_{\varepsilon_1 \downarrow 0} \int_R (R^0_{\lambda - i\varepsilon_1} - R^0_{\lambda + i\varepsilon_1})\, V \left(I - s\text{-}\lim_{\varepsilon_2 \downarrow 0} \int_R R_{\lambda + i\varepsilon_2} V\, dE^0_\mu \right) dE^0_\lambda\, \psi\,. \tag{43}$$

Our aim is to transform this expression into

$$R\,\psi = s\text{-}\lim_{\varepsilon_1 \downarrow 0}\; s\text{-}\lim_{\varepsilon_2 \downarrow 0} \int_R (R^0_{\lambda - i\varepsilon_1} - R^0_{\lambda + i\varepsilon_1})\, (V - V\, R_{\lambda + i\varepsilon_2}\, V)\, dE^0_\lambda\, \psi \tag{42}$$

which is the mathematically precise analogue of the formal expression '(42)'.

We shall begin transforming (43) into (42) by first exchanging the limit $\varepsilon_2 \downarrow 0$ with the spectral integral. The necessary and sufficient condition for this is established in

Lemma 4: Under the hypothesis of conditions (θ), (A), (B) and (C) the necessary and sufficient condition for the validity for all $\psi \in \mathcal{D}$ of

$$\int_R (R^0_{\lambda - i\varepsilon_1} - R^0_{\lambda + i\varepsilon_1})\, V \left[s\text{-}\lim_{\varepsilon_2 \downarrow 0} \int_R R_{\mu + i\varepsilon_2}\, V\, dE^0_\mu \right] dE^0_\lambda\, \psi =$$

$$= s\text{-}\lim_{\varepsilon_2 \downarrow 0} \int_R (R^0_{\lambda - i\varepsilon_1} - R^0_{\lambda + i\varepsilon_1})\, V \left(\int_R R_{\mu + i\varepsilon_2}\, V\, dE^0_\mu \right) dE^0_\lambda\, \psi \tag{44}$$

is that for all $\psi \in \mathcal{D}$

$$s\text{-}\lim_{\varepsilon_2 \downarrow 0} \int_0^\infty e^{-\varepsilon_1 t} [U_t^*\, V\, (\Omega_+ - \Omega_{\varepsilon_2})\, U_t + U_t\, V\, (\Omega_+ - \Omega_{\varepsilon_2})\, U_t^*]\, \psi\, dt = 0 \tag{D}$$

where

$$\Omega_\varepsilon = \varepsilon \int_{-\infty}^0 e^{\varepsilon t}\, V_t^*\, U_t\, dt \qquad (\varepsilon > 0)\,.$$

Proof of Lemma 4: We observe first that, by virtue of (35), equation (44) is equivalent to

$$s\text{-}\lim_{\varepsilon_2 \downarrow 0} \int_R (R^0_{\lambda - i\varepsilon_1} - R^0_{\lambda + i\varepsilon_1})\, V\, (\Omega_+ - \Omega_{\varepsilon_2})\, dE^0_\lambda\, \psi = 0\,. \tag{45}$$

To establish (45), we show that the left-hand side can be transformed into an integral over t with the help of the formula

$$\int_R R^0_{\lambda \pm i\varepsilon_1}\, V\, (\Omega_+ - \Omega_{\varepsilon_2})\, dE^0_\lambda\, \psi = i \int_0^{\pm\infty} e^{\mp \varepsilon_1 t}\, U_t\, V\, (\Omega_+ - \Omega_{\varepsilon_2})\, U_t^*\, \psi\, dt\,. \tag{46}$$

This formula is obtained from theorem 3 by writing its right-hand side as

$$i \int_0^{\pm\infty} e^{\mp \varepsilon_1 t}\, U_t\, V\, (\Omega_+ - \Omega_{\varepsilon_2})\, U_t^*\, \psi\, dt$$

$$= i \int_0^{\pm\infty} e^{\mp \varepsilon_1 t}\, U_t\, V\, (\Omega_+ - \Omega_{\varepsilon_2}) \left(\int_R e^{i\lambda t}\, dE^0_\lambda\, \psi \right) dt\,. \tag{47}$$

The applicability of theorem 3 depends on the following property

$$\|V\, (\Omega_+ - \Omega_{\varepsilon_2})\, \psi\| \leqslant \alpha\, \|H_0\, \psi\| + \beta\, \|\psi\|\,, \qquad \psi \in \mathcal{D};\, \alpha, \beta \geqslant 0\,. \tag{48}$$

This inequality can be verified by noticing that the condition (θ) implies that

(i) $\psi \in \mathcal{D} \Rightarrow \Omega_\varepsilon \psi \in \mathcal{D}$,

(ii) $\| V \Omega_\varepsilon \psi \| \leqslant M (\| H_0 \psi \| + \| \psi \|)$

with M independent of ε.

The inequality (48) implies also the existence of the integral in (47).

Inserting (46) into (45) leads to

$$\text{s-}\lim_{\varepsilon_2 \downarrow 0} \int_0^\infty e^{-\varepsilon_1 t} \left[U_t^* V (\Omega_+ - \Omega_{\varepsilon_2}) U_t + U_t V (\Omega_+ - \Omega_{\varepsilon_2}) U_t^* \right] \psi \, dt = 0 \tag{D}$$

and this proves the lemma 4.

The second step in transforming (43) is the reduction of the double spectral integral to a single spectral integral. For this we need the formula

$$\int_{\mathbf{R}} R^0_{\lambda \pm i\varepsilon_1} V \left(\int_{\mathbf{R}} R_{\mu + i\varepsilon_2} V \, dE^0_\mu \right) dE^0_\lambda \psi$$
$$= \int_{\mathbf{R}} R^0_{\lambda \pm i\varepsilon_1} V R_{\lambda + i\varepsilon_2} V \, dE^0_\lambda \psi \, . \tag{49}$$

This formula is obtained with the help of

Lemma 5: Let $\mathcal{H}$ be a separable Hilbert space and F_λ a spectral family of projection operators. Suppose further that $u(\lambda)$ and $v(\lambda)$ are two bounded operator valued functions u: $(a, b) \to \mathfrak{B}(\mathcal{H})$, v: $\mathbf{R} \to \mathfrak{B}(\mathcal{H})$ where $(a, b) \subset \mathbf{R}$ may be finite or infinite, such that

(1) $$J = \int_a^b u(\lambda) \left(\int_{\mathbf{R}} v(\mu) \, dF_\mu \right) dF_\lambda \psi \tag{50}$$

exists for $\psi \in \mathcal{H}$.

(2) on any finite interval $K \subset (a, b)$

(a) $\sup_{\lambda \varepsilon K} \| u(\lambda) \| = M(K) < \infty$,

(b) there exist $L(K) < \infty$ and $\alpha(K) > 1/2$ such that for all $\lambda, \mu \in K$: $\| v(\lambda) - v(\mu) \| \leqslant L(K) \, |\lambda - \mu|^{\alpha(K)}$.

Then

$$J' = \int_a^b u(\lambda) \, v(\lambda) \, dF_\lambda \psi$$

exists and

$$J = J' \, .$$

Proof of Lemma 5: It suffices to prove the lemma 5 for finite intervals (a, b). For infinite intervals we take the limit either $a \to -\infty$ or $b \to +\infty$ or both and since this limit exists for J it exists also for J' and is equal to it.

We have from the definition of the spectral integral

$$J = s\text{-}\lim_{|\pi|\to 0} \sum_{i=1}^{n} u(\lambda_i') \left(\int_{R} v(\mu) \; dF_\mu \right) F_{\Delta_i} \psi \tag{51}$$

where

$$\pi = \{a = \lambda_0 < \lambda_1 < \cdots < \lambda_n = b\} ,$$

$$F_{\Delta_i} = F_{\lambda_i} - F_{\lambda_{i-1}} \quad \text{and} \quad \lambda_i' \in (\lambda_{i-1}, \lambda_i) .$$

Since

$$\int_{R} v(\mu) \, dF_\mu \, (F_{\lambda_i} - F_{\lambda_{i-1}}) \, \psi = \int_{\lambda_{i-1}}^{\lambda_i} v(\mu) \, dF_\mu \, \psi ,$$

we obtain for (51)

$$J = s\text{-}\lim_{|\pi|\to 0} \sum_{i=1}^{n} u(\lambda_i') \int_{\lambda_{i-1}}^{\lambda_i} v(\mu) \, dF_\mu \, \psi .$$

We would like to show that this is equal to

$$J = s\text{-}\lim_{|\pi|\to 0} \sum_{i=1}^{n} u(\lambda_i') \; v(\lambda_i') \; F_{\Delta_i} \psi$$

or equivalently that

$$s\text{-}\lim_{|\pi|\to 0} \left[\sum_{i=1}^{n} u(\lambda_i') \int_{\lambda_{i-1}}^{\lambda_i} v(\mu) \, dF_\mu \, \psi - \sum_{i=1}^{n} u(\lambda_i') \; v(\lambda_i') \; F_{\Delta_i} \, \psi \right] = 0 .$$

We shall estimate the norm of the left by

$$\alpha_\pi \equiv \| \sum_{i=1}^{n} u(\lambda_i') \left[\int_{\lambda_{i-1}}^{\lambda_i} v(\mu) \, dF_\mu \, \psi - v(\lambda_i') \, F_{\Delta_i} \psi \right] \| \leqslant$$

$$\leqslant \sum_{i=1}^{n} \| \int_{\lambda_{i-1}}^{\lambda_i} u(\lambda_i') \, [v(\mu) - v(\lambda_i')] \, dF_\mu \, \psi \| \equiv \sum_{i=1}^{n} S_i .$$

Let $w_\mu(\lambda) \equiv u(\mu) \, [v(\lambda) - v(\mu)]$. It follows that

$$\|w_\mu(\lambda_1) - w_\mu(\lambda_2)\| = \|u(\mu) \, [v(\lambda_1) - v(\lambda_2)\| \leqslant$$

$$\leqslant \|u(\mu)\| \, \|v(\lambda_1) - v(\lambda_2)\| \leqslant M \; L \; |\lambda_1 - \lambda_2|^\alpha$$

and

$$\|w_\mu(\lambda)\| \leqslant \|u(\mu)\| \, \|v(\lambda) - v(\mu)\| \leqslant M \; L \; |\lambda - \mu|^\alpha .$$

where L is defined as $L(K)$ for $K = (a, b)$, and similarly for M and α.

We can now apply a theorem of Birman and Solomjak (cf. reference [4]) which gives the following estimate for S_i:

$$S_i = \| \int_{\lambda_{i-1}}^{\lambda_i} w_{\lambda_i'} (\mu) \, dF_\mu \, \psi \| \leqslant \left[\frac{2}{1 - 2^{1/2-\alpha}} L \, (\lambda_i - \lambda_{i-1})^\alpha + M \, L \, (\lambda_i - \lambda_{i-1})^\alpha \right] \; \| F_{\Delta_i} \psi \| .$$

Consequently

$$\begin{aligned}
\alpha_\pi &\leqslant \text{const.} \sum_{i=1}^{n} (\lambda_i - \lambda_{i-1})^\alpha \, \|F_{\Delta_i} \psi\| \\
&\leqslant \text{const.} \sup_{1 \leqslant j \leqslant n} \{(\lambda_j - \lambda_{j-1})^{\alpha - 1/2}\} \sum_{i=1}^{n} (\lambda_i - \lambda_{i-1})^{1/2} \, \|F_{\Delta_i} \psi\| \\
&\leqslant \text{const.} \, |\pi|^{\alpha - 1/2} \left(\sum_{i=1}^{n} [(\lambda_i - \lambda_{i-1})^{1/2}]^2 \right)^{1/2} \left(\sum_{i=1}^{n} \|F_{\Delta_i} \psi\|^2 \right)^{1/2} \\
&\leqslant \text{const.} \, |\pi|^{\alpha - 1/2} (b-a)^{1/2} \, \|\psi\|^2
\end{aligned}$$

where the third inequality is obtained by applying the inequality of Schwarz. It follows that α_π converges to zero with $|\pi| \to 0$, and thus lemma 5 is proved.

Equation (49) is easily obtained from lemma 5 by setting $u(\lambda) = R^0_{\lambda \pm i\varepsilon_1} V$, $v(\lambda) = R_{\lambda + i\varepsilon_2} V$ and by noticing that

$$\| R_{\lambda + i\varepsilon_2} V - R_{\mu + i\varepsilon_2} V \| \leqslant \text{const.} \, |\lambda - \mu| \, .$$

We collect the result in

Theorem 8:

If (θ), (A), (B), (C) and in addition condition (D) are satisfied, then for all $\psi \in \mathfrak{D}$

$$R\psi = s\text{-}\lim_{\varepsilon_1 \downarrow 0} \; s\text{-}\lim_{\varepsilon_2 \downarrow 0} \int_{\mathbf{R}} (R^0_{\lambda - i\varepsilon_1} - R^0_{\lambda + i\varepsilon_1}) \, (V - V\, R_{\lambda + i\varepsilon_2} V) \, dE^0_\lambda \psi \, . \tag{42}$$

This equation represents the translation of the heuristic formula '(42)' into a meaningful mathematical expression.

The condition for its validity is the additional property (D). We do not know whether (D) is an independent condition or whether it can be derived from the others, in particular from (θ) and (A). We have only some minor results in this direction which we give as

Theorem 9:

(a) If (θ) and (A) are satisfied and if in addition s-lim $V\, \Omega_\varepsilon \psi$ with $\varepsilon \downarrow 0$ exists for all $\psi \in \mathfrak{D}$, then condition (D) is satisfied.

(b) If (θ), (A) and (B) are satisfied and $V\, R^0_z$ is compact for some non-real z, then condition (D) is also satisfied.

The condition that $V\, R^0_z$ be compact for non-real z is verified for a large class of local potentials for the Schrödinger operator $H_0 = -\Delta/(2\,m)$[19].

Proof:

(a) The vectors $(\Omega_+ - \Omega_\varepsilon)\, U_t \psi$ belong to $\mathfrak{D}$ for $\psi \in \mathfrak{D}$ and converge strongly to zero with $\varepsilon \downarrow 0$. From the hypothesis it follows that $V\, (\Omega_+ - \Omega_\varepsilon)\, U_t \psi$ tends to a limit with $\varepsilon \downarrow 0$. Since V is symmetric, this limit is zero.

By applying (48), one obtains

$$\|e^{-\varepsilon_1 t} U_t^* V (\Omega_+ - \Omega_{\varepsilon_2}) U_t \psi\| \leqslant e^{-\varepsilon_1 t} (\alpha \|H_0 \psi\| + \beta \|\psi\|) .$$

Since this is integrable, Lebesgue's theorem (cf. section 2) applies and gives

$$\text{s-}\lim_{\varepsilon_2 \downarrow 0} \int_0^\infty e^{-\varepsilon_1 t} U_t^* V (\Omega_+ - \Omega_{\varepsilon_2}) U_t \psi \, dt = 0 .$$

The second integral of (D) is shown to be zero in a similar way. This proves part (a) of the theorem.

(b) Let $\psi \in \mathfrak{D}$. Using first condition (θ) and then lemma 1, one gets

$$\|V V_t^* U_t \psi\| \leqslant \alpha \|H U_t \psi\| + \beta \|\psi\| \leqslant \alpha' \|H_0 \psi\| + \beta' \|\psi\| .$$

Thus $V V_t^* U_t \psi$ is uniformly bounded. We shall also see that it converges strongly as $t \to -\infty$. It then follows that

$$\chi_\varepsilon = \varepsilon \int_{-\infty}^0 e^{\varepsilon t} V V_t^* U_t \psi \, d t$$

converges strongly as $\varepsilon \downarrow 0$ (see for instance lemma 6 of reference [13]). But since V is symmetric (i.e. $V \subseteq V^*$ and V^* is closed), one has $\chi_\varepsilon = V \Omega_\varepsilon \psi$. Hence, according to part (a), condition (D) is satisfied.

To show the strong convergence of $V V_t^* U_t \psi$, we notice that $(V_t^* U_t - \Omega_+) \psi \in \mathfrak{D}$. Hence condition (θ) implies

$$\|V (V_t^* U_t - \Omega_+) \psi\| \leqslant \alpha \|H (V_t^* U_t - \Omega_+) \psi\| + \beta \|(V_t^* U_t - \Omega_+) \psi\| .$$

The second term on the right-hand side converges to zero with $t \to -\infty$ as a consequence of (A). For the first term we write

$$\begin{aligned} \|H (V_t^* U_t - \Omega_+) \psi\| &= \|(H_0 + V) U_t \psi - V_t H \Omega_+ \psi\| = \\ &= \|H_0 U_t \psi - V_t \Omega_+ H_0 \psi + V U_t \psi\| \leqslant \|(V_t^* U_t - \Omega_+) H_0 \psi\| + \\ &+ \|V R_z^0 U_t (H_0 - z) \psi\| . \end{aligned}$$

In the last member of this inequality, the first term converges to zero because of (A). The second term also converges to zero because $V R_z^0$ is compact by hypothesis and because $U_t (H_0 - z) \psi$ converges weakly to zero with $t \to -\infty$ as a consequence of condition (B).

Thus we have shown that

$$\text{s-}\lim_{t \to -\infty} V V_t^* U_t \psi = V \Omega_+ \psi$$

and this completes the proof of theorem 9.

7. Conclusion and Final Remarks

We conclude with a few remarks on the significance of the stationary state formalism for possible future generalisations of scattering theory.

It is by now generally known that condition (A), which is the basis for the time-dependent scattering theory, is too strong a condition, since it excludes some physically important cases. For instance the Coulomb potential does not satisfy condition (A).

The Coulomb case is a mild example of the persistence of interactions at $t \to \pm \infty$. Much stronger examples of this kind are known from field theoretic models of scattering systems.

It is suggestive to remark that we have *not* shown the *equivalence* of the stationary formalism and the time-dependent one, we have only shown that the former can be derived from the latter. It seems not impossible that the formulae for stationary scattering theory, suitable generalized, can be the starting point of a scattering theory which is adequate on the other side of the Coulomb barrier and may lead to a theory of scattering with dressing transformations [20, 21]. The results so far obtained along this line are promising and they will be the object of a future communication.

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