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Arrival time observables in quantum mechanics

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ABSTRACT. — Arrival time observables are defined, which jointly measure the arrival time and some arrival event of a quantum system. Arrival times may be constructed from an arbitrary contraction semigroup describing the absorption process and an arbitrary observable in the « exit space », which is defined as a certain Hilbert space canonically associated with the semigroup. The connection with the covariant observable approach to arrival time measurements is given by scattering theory. The example of the arrival at the origin of a particle on the half line with internal degrees of freedom is treated in detail.

RÉSUMÉ. — On définit des observables de temps d'arrivée, qui mesurent à la fois le temps d'arrivée et un événement d'arrivée pour un système quantique. On peut construire des temps d'arrivée à partir d'un semi-groupe de contraction arbitraire décrivant le processus d'absorption, et d'un observable arbitraire dans « l'espace de sortie », qui est défini comme un certain espace de Hilbert canoniquement associé au semi-groupe. La relation avec le traitement de la mesure des temps d'arrivée au moyen d'observables covariants est donnée par la théorie de la diffusion. On traite en détail l'exemple de l'arrivée à l'origine d'une particule sur une demi-droite, possédant des degrés de liberté internes.

I. INTRODUCTION

There is a strange discrepancy between many theoretical accounts of measurement in quantum mechanics and the typical measurement carried out in a laboratory. On the one hand, every counter clicks at a certain time, and frequently these times are quite important for the evaluation of an experiment, e. g. a correlation experiment. On the other hand, operators describing the probability that a counter responds during a given time interval are rarely discussed in quantum mechanics textbooks. The reason for this deficiency is probably that a selfadjoint « time operator » canonically conjugate to the Hamiltonian cannot exist due to the semiboundedness of the Hamiltonian. It was therefore an important step towards a more realistic quantum mechanical description of actual experiments to realize [*1*] [*2*] that a yes-no measurement in quantum mechanics is not necessarily given by a projection but possibly by any operator between zero and one. In this slightly generalized framework « time observables » which are covariant with respect to the time evolution can easily be constructed.

In quantum mechanics time occurs in two distinct but related ways, each of which suggests a different formal description of the time of response of a counter. The first may be called the « kinematical » view of time evolutions. Consider experiments composed of a preparing device mathematically represented by a density matrix W and a measuring device represented by an operator F. We assume that the macroscopic descriptions of these devices also specify how and when to trigger them so that it makes sense to speak about « the same measuring device triggered t seconds later ». This modified device is then represented by $F' = U_t^* F U_t$, where U_t is the unitary time evolution operator. Of course, we may equivalently trigger the preparing device t seconds earlier, which is the operation described by the Schrödinger picture of time evolution. Both preparation and measuring process take a finite time, so that it makes no sense, for example, to talk about the « simultaneous » rather than the « joint » measurement of two observables. In this kinematical view of time evolution neither the state nor the observable change as time goes by. The Heisenberg and Schrödinger time evolutions merely refer to a change of the time interval between the triggering of preparing and measuring process just as a unitary representation of the Poincaré or Galilei group describes a change in the relative space-time orientation of these processes. Now consider a counter which by itself is in a stable state. Upon interaction with a microsystem it may change its macroscopic state and emit a « click ». We shall be interested only in the first click, so it does not matter whether the counter is recharged or not. According to the general principles of quantum mechanics the probability $p(\Theta)$ that the counter clicks during the time interval Θ for systems prepared in the state W must be of the form $p(\Theta) = \operatorname{tr} WF(\Theta)$ for some operator $0 \leqslant F(\Theta) \leqslant 1$. Thus the counter is described by an observable, or positive operator valued measure, on the time axis. Suppose now that we initialize the counter t seconds later. Since we have assumed that it is in a stable state as long as it is left alone, this only means a different setting of the clock by which the clicks are labelled, i. e. the measure p is shifted by t seconds. Since this holds for all states W, F must be a *covariant observable* in the sense that $U_t^* F(\Theta) U_t = F(\Theta + t)$ [*2*]. This idea of covariant observables easily extends to larger symmetry groups and homogeneous parameter spaces. For example, one may use it to define quantum analogs of arrival time and arrival location of a classical relativistic or non-relativistic particle at a screen [*3*]. Due to the high symmetry of the screen situation one may even characterize a unique « sharpest » or « ideal » screen observable.

The second view of time evolution might called « dynamical ». On this view, the state of the system « at time t » really changes with time as the system « propagates » in its environment. This is particularly suggestive if the environment, represented e. g. by external fields in the Hamiltonian, is time-dependent itself. It is clearly implicit in the usual treatment of time-dependent external fields that the Hamiltonian at time t determines the evolution of states at this time instant. Instantaneous interaction, however, can occur in physics only as an approximation to a more complete description. In the case of external electromagnetic fields this more comprehensive theory would be quantum electrodynamics. It is impossible at the moment to apply this theory to the situations in which the standard description of external fields is usually applied. An important simplification at the root of the external field picture is that the electromagnetic field is described by a purely classical theory. Since the time evolution of the total system (external field plus quantum system) is taken to be reversible it then follows that the field obeys a closed set of evolution equations independent of the state of the quantum system. The solutions of these equations determine a time dependent modification of the Hamiltonian of the quantum subsystem. The interaction is thus only in one direction, and one systematically neglects the contribution to the field due to radiation by the quantum system as well as the energy loss of the quantum system due to radiation damping. It is possible to include some effects of radiation damping into this description [*4*]. In this case the dynamics of the total system necessarily becomes irreversible in the sense that pure states may evolve into mixed states.

A full quantum electrodynamical description of the interaction between system and measuring device would also contain relativistic retardations, so that any measurement necessarily takes a non-zero time interval. Using such measurements it is impossible to determine the state of the system « at time t ». This concept only makes sense in a non-relativistic approximation, where retardations can be neglected so that there may be sufficiently many measurements which require only a negligible time of interaction. The state of the system « at time t » may then be defined in terms of the responses of the system to such almost instantaneous probes. In a relativistic theory this concept loses its meaning and must be replaced by the concept of local states, i. e. the restrictions of the state of the total system to the algebras of observables localized in different space time regions [5]. The instantaneous interactions of the non-relativistic theory are then to be replaced by localized operations [6] [7]. The study of relativistically localized arrival events in the framework of algebraic quantum field theory would be an interesting extension of the present study, which must be left to a later occasion.

In this paper we shall develop a way to describe the arrival of a non-relativistic system at a macroscopic counter in the spirit of the dynamical view of time evolution. As in the description of external fields those properties of the macroscopic object (counter or field), which are relevant for the evolution of the quantum system will be assumed not to be influenced by the quantum system. The irreversibility of the absorption at a counter forces the modified quantum evolution to be non unitary. In connection with complex « optical » potentials such non-unitary time evolutions have been used for a long time. The interpretation in terms of survival and capture probabilities can be found e. g. in [2, chapter 7.4]. The main new element introduced in this paper is the « exit space » associated with any continuous contraction semigroup on a Hilbert space, which describes in a natural way the quantum states at arrival time.

This space and the concept of quantum arrival times will be introduced in section II. In section III the relation to covariant time observables, i. e. to the notion of arrival times appropriate to the kinematical view will be investigated. The example in the final section IV serves to illustrate this connection as well as some of the general properties of arrival times.

II. ARRIVAL TIME OBSERVABLES

Consider a microsystem in an environment containing several macroscopic objects like counters or absorbing walls. This is a frequently encountered situation, but it is usually quite impossible to give a fully quantum mechanical description of such macroscopic objects and their interaction with a microsystem. Therefore we want to give an idealized description of the microsystem up until the time when it becomes absorbed by one of the walls or counters. Our first assumption is that the maps S_t ($t \in \mathbb{R}^+$) taking the density matrix W of an ensemble of microsystems at time zero to the density matrix $W_t = S_t(W)$ at a later time t form a dynamical semigroup [2]. This excludes time dependent external fields but also neglects the influence on the microsystem of the state changes of the counters due to the interaction with the microsystem itself. Thus the counters and walls in the environment of the microsystem will only enter the theory as modifications of the generator of the dynamical semigroup S. Since we want to study absorption we shall not assume that this semigroup preserves normalization. Instead, $0 \leqslant \mathrm{tr}\, W_t \leqslant 1$ will be interpreted as the probability that a system survives at least until time t.

Our second assumption will be that the dynamical semigroup introduces as little randomness as possible in the sense that it takes pure states to pure states (with possibly smaller normalization). This assumption of « purity » also plays an important role in Davies's theory of quantum stochastic processes and greatly simplifies the mathematical analysis. It excludes, for example, the description of the energy exchange between a gas particle and a hot wall. As a consequence of these two assumptions we can write the time evolution as $W_t = S_t(W) = B_t W B_t^*$ with $B_t = \exp(-iLt)$ a semigroup of contractions on the Hilbert space $\mathfrak{H}$ of the microsystem.

By our above interpretation of the normalization $\mathrm{tr}\, W_t$ the probability for the system to be absorbed during the time interval $[s, t]$ is given by $\mathrm{tr}\, W\hat{G}[s, t]$, where $\hat{G}(\cdot)$ denotes the positive operator valued measure on the positive time axis $\mathbb{R}^+$ given by $\hat{G}[0, t) = 1 - B_t^* B_t$. By construction, $\hat{G}$ is a covariant observable with respect to the semigroup B, i. e. for any Borel set $\Theta \subset \mathbb{R}^+$ and any $t \in \mathbb{R}^+$ we have $B_t^* \hat{G}(\Theta) B_t = \hat{G}(\Theta + t)$.

Thus any contraction semigroup B determines a natural arrival time observable $\hat{G}$. However, one is usually not only interested in the arrival time distribution but also in the probability of certain events at that time, e. g. the location at which the particle has reached the boundary. It is well known how to calculate such probabilities for first passage and general stopping times of a classical diffusion process: in this case one simply considers for each sample path the state of the system at arrival time. This state will be a point on the boundary, so that the « observables at arrival time » are given by functions on the boundary. In the quantum case it is not so clear how the state « at arrival time » may be defined, even if one accepts the notion of states « at time t ». The source of this difficulty is that measurements at different times need no longer be compatible so that it is impossible to define probabilities of sample paths. It is clear that a quantum observable at arrival time will typically not be jointly measurable with any observable at a fixed time. On the other hand such an observable should be jointly measurable with the above arrival time observable $\hat{G}$. It turns out that there is a natural construction for both states and observables « at arrival time » associated with an arbitrary contraction semigroup B. This construction will now be presented. The rest of the paper will be devoted to the question to what extent this construction is in accordance with the intuitions about arrival times derived from classical diffusions.

Since $B_t = \exp(-iLt)$ is a contraction semigroup,

$$\Phi \mapsto -\frac{d}{dt} \| B_t \Phi \|^2 |_{t=0} \tag{1}$$

defines a positive semidefinite quadratic form on dom (L). Its value at

$\Phi \in \operatorname{dom} L$ is interpreted as the probability density for arrival at time zero for systems prepared in the pure state Φ. Let $\mathfrak{K}$ denote the Hausdorff-completion of this pre-Hilbert space and $j : \operatorname{dom} L \to \mathfrak{K}$ the canonical embedding. $\mathfrak{K}$ is a Hilbert space, whose inner product is defined on the dense set $j(\operatorname{dom} L) \subset \mathfrak{K}$ by

$$\langle j\Phi, j\Psi \rangle = \langle iL\Phi, \Psi \rangle + \langle \Phi, iL\Psi \rangle. \tag{2}$$

This space $\mathfrak{K}$ describes the possible states of the system upon arrival in much the same way as $\mathfrak{H}$ describes the usual states of the system. It will be shown below that this interpretation depends only on eq. (2) so that we shall call any Hilbert space $\mathfrak{K}$ with a map $j : \operatorname{dom} L \to \mathfrak{K}$ satisfying (2) an *exit space* for the semigroup B. The special exit space constructed above by completion may then be identified with the closed subspace of $\mathfrak{K}$ generated by $j(\operatorname{dom} L)$ and will be called the *minimal* exit space for B. It is worthwile to note that it suffices to check eq. (2) for Φ and Ψ in a core for L, since this relation automatically carries over to the closure of L.

For each $\Phi \in \operatorname{dom} L$ consider the function $J\Phi : \mathbb{R}^+ \to \mathfrak{K}$ given by $(J\Phi)(t) = j(B_t\Phi)$. Then

$$\int_0^\infty dt \, \| J\Phi(t) \|^2 = - \int_0^\infty dt \frac{d}{dt} \| B_t\Phi \|^2 - \lim_{t\to\infty} \| B_t\Phi \|^2 \leqslant \| \Phi \|^2 . \tag{3}$$

where the limit exists by contractivity of B_t. This bound shows that J extends to a contraction $J : \mathfrak{H} \to \mathfrak{L}^2(\mathbb{R}^+, dt ; \mathfrak{K}) \equiv \mathfrak{L}^2(\mathbb{R}^+, dt) \otimes \mathfrak{K}$. Note that the space $\mathfrak{L}^2(\mathbb{R}^+, dt)$ carries a natural time observable G such that $G(\Theta)$ is the operator of multiplication with the characteristic function of Θ. G is related to the arrival time observable $\hat{G}$ defined above via $\hat{G}(\Theta) = J^*(G(\Theta) \otimes \mathbb{1})J$. Clearly, $G(\cdot) \otimes \mathbb{1}$ can be measured together with any observable of the form $\mathbb{1} \otimes F(\cdot)$. We shall call any such observable F, i. e. any measure on a measurable space X, whose values $F(\sigma)$ for $\sigma \subset X$ are positive operators on $\mathfrak{K}$ with $0 \leqslant F(\sigma) \leqslant \mathbb{1}$ an *exit observable.*

Typically, X will be some space of exit parameters like the surface of a screen or a set labelling a collection of counters. Then for measurable $\Theta \subset \mathbb{R}^+$ and $\sigma \subset X$

$$\hat{F}(\Theta \times \sigma) = J^*G(\Theta) \otimes F(\sigma)J \tag{4}$$

defines an observable $\hat{F}$ over $\mathbb{R}^+ \times X$ jointly measuring the arrival time $t \in \mathbb{R}^+$ and the exit parameter $x \in X$. We shall call $\hat{F}$ the *arrival time observable* associated with F. The set of arrival time observables thus constructed for a given contraction semigroup B does not depend on the choice of the (possibly non-minimal) exit space $(\mathfrak{K}, j)$. For the construction of $\hat{F}$ it suffices to know the sesquilinear forms F_σ on dom L given $F_\sigma(\Phi, \Psi) = \langle j\Phi, F(\sigma)j\Psi \rangle$ for any operator $F(\sigma) \in \mathfrak{B}(\mathfrak{K})$. Then for $\Phi, \Psi \in \operatorname{dom} L$

$$\langle \Phi, \hat{F}(\Theta \times \sigma)\Psi \rangle = \int_{t\in\Theta} F_\sigma(B_t\Phi, B_t\Psi)dt . \tag{5}$$

This formula is also useful for checking the covariance property $B_t^* \hat{F}(\Theta \times \sigma) B_t = \hat{F}((\Theta + t) \times \sigma)$ for $t \geqslant 0$ and $\Theta \subset \mathbb{R}^+$, which will be needed in section III.

In general the observable $\hat{F}$ is not normalized, i. e.

$$\hat{F}(\mathbb{R}^+ \times X) = J^* \mathbb{1} \otimes F(X) J \neq \mathbb{1},$$

even if $F(X) = \mathbb{1}$. In fact, $\operatorname{tr} W \hat{F}(\mathbb{R}^+ \times X)$ is the probability for systems in the initial state W to be detected at all. Assuming $F(X) = \mathbb{1}$, the operator J^*J and its spectral resolution provide an overview over the chances for a system to be detected. Let $\mathfrak{H}_0$, $\mathfrak{H}'$, and $\mathfrak{H}_1$ denote the spectral subspaces for the subsets $\{0\}$, $(0, 1)$, and $\{1\}$ of the spectrum of J^*J. It is clear from the estimate (3) that $\mathfrak{H}_0$ is the largest subspace on which B_t is unitary for some and hence for all $t > 0$. Systems in a pure state $\varphi \in \mathfrak{H}_0$ are never detected, in contrast to systems with $\varphi \in \mathfrak{H}_1$ which are eventually detected with probability one. By definition, J restricted to $\mathfrak{H}_1$ is an isometry. Moreover, it is clear from the definition that J intertwines B_t and the shift on $\mathfrak{L}^2(\mathbb{R}^+, dx; \mathfrak{K})$. Hence the dilation of the semigroup $B_t \upharpoonright \mathfrak{H}_1$ is isomorphic to the shift on $\mathfrak{L}^2(\mathbb{R}, dx; \mathfrak{K})$ (compare [*2*, chapter 7.3]).

In the following example B, $\mathfrak{K}$, F, and hence $\hat{F}$ have a simple intuitive interpretation. Some of its aspects will be further elaborated in section IV.

EXAMPLE. — Particle in a region of $\mathbb{R}^d$.

Let $\Omega \subset \mathbb{R}^d$ be a region with smooth boundary $\partial\Omega$. We want to describe a particle (with spin 0 and mass 1) which moves freely in the interior of Ω but may be absorbed at the boundary. The Hilbert space of the system is $\mathfrak{H} = \mathfrak{L}^2(\Omega, dx)$. Let L_0 be the operator $L_0\psi = -\frac{1}{2}\Delta\psi$ on the domain of smooth functions $\psi \in \mathfrak{H}$ with compact support contained in the interior of Ω. We take « free motion in the interior of Ω » to mean that the generator L of B_t must be an extension of L_0. There are many extensions of L_0, some of which arise from identifying different pieces of $\partial\Omega$. Simple absorption is described by boundary conditions, which depend only on the boundary data of ψ at a single point $x \in \partial\Omega$:

$$\vec{n}(x) \cdot \nabla\psi(x) = a(x)\psi(x) \qquad \text{for} \quad x \in \partial\Omega,\ \psi \in \operatorname{dom} L \tag{6}$$

where $a : \partial\Omega \to \mathbb{C}$ is smooth and $\vec{n}$ denotes the unit normal of $\partial\Omega$. (For the sake of notational simplicity we have excluded the Dirichlet boundary condition corresponding to $a = \infty$, cf. section IV). Then we have for smooth functions $\psi \in \operatorname{dom} L$ with a smooth extension to a neighbourhood of Ω:

$$\begin{aligned} -\frac{d}{dt}\| B\psi \|^2 &= \langle iL\psi, \psi \rangle + \langle \psi, iL\psi \rangle = \frac{1}{2i}\int_\Omega dx \nabla \cdot \{ \psi^*\nabla\psi - \psi\nabla\psi^* \} \\ &= \int_{\partial\Omega} df\, \mathscr{Im}\{ \psi^* \vec{n} \cdot \nabla\psi \} = \int_{\partial\Omega} df\, \mathscr{Im}(a) \, | \psi |^2 , \end{aligned} \tag{7}$$

where df denotes the surface element of $\partial\Omega$. (One can show that such ψ will be a core for L). Directly from this formula one sees that contraction generators are characterized by $\mathscr{I}m\, a \geqslant 0$ on $\partial\Omega$ and that the exit space is naturally identified with $\mathfrak{K} = \mathfrak{L}^2(\partial\Omega, \mathscr{I}m\,(a)df)$. The exit observable F measuring the « arrival location » of the particle is the « position » observable in $\partial\Omega$ acting by multiplication.

Formula (7) suggests that the absorption is proportional to $\mathscr{I}m\, a$, and could thus be made arbitrarily large. However, this is false, since $\mathscr{I}m\, a \to \infty$ is the ideally reflecting Dirichlet boundary condition. This phenomenon, which will emerge more clearly in section IV, can be paraphrased by saying that in quantum mechanics increasing absorption implies increasing reflection so that absorption can never be total (compare [*2*, chapter 7.4]).

III. REVERSIBLE AND IRREVERSIBLE TIME EVOLUTION

It is generally held that the kinematical properties of an elementary particle are summarized in an irreducible projective representation of the Galilei or Poincaré group. As described in the introduction we have adopted the view that the « free » time evolution contained in this group must in general be modified to an irreversible evolution in the presence of counters. So far we have not used the free time evolution at all but only the « modified » one. How then can we justify the claim that this modified evolution still describes, say, electrons? The same question arises already in the ordinary description of interactions via potentials: if we define an electron as an irreducible representation of the Galilei or Poincaré group, in what sense does the Hydrogen Hamiltonian then describe electrons?

We can give two more or less standard answers. As pointed out above it is inherent in the description via (possibly time dependent) potentials that there is a sufficient set of measurements of short duration for identifying the state of the system « at time t ». The first answer is that these almost instantaneous measurements also suffice to identify the particle. In the dynamical view of time evolution it is thus possible to speak about « the same particle » in dynamically different environments. Moreover, the description of a complex environment can be obtained by adding the potentials describing the influence of the various external sources. In the case at hand we may introduce « the same counter » into different environments by adding the same non-hermitian term to the generator of the time evolution. Similarly we may construct observables for arbitrary arrays of counters, once the description of the individual counters is given (see below).

The second answer to the identity of particles in interaction is more in the spirit of the kinematical view of time evolution. On this view, considering the electron as a well-defined subsystem of the hydrogen atom is as impossible as separating an electron from its surrounding photon cloud. Only when proton and electron are widely separated, i. e. in the limit of scattering theory, the Galilei or Poincaré symmetry of the constituents becomes exact and the particle concept is applicable. We shall see below that in a scattering limit the arrival time observables defined in section II become covariant observables for the « free » reversible time evolution. Hence in this limit the concept of arrival time observables appropriate to the dynamical view coincides with the concept appropriate to the kinematical view of time evolution.

We begin by studying arrays of counters. Let H denote the Hamiltonian of the reversible time evolution. For simplicity we assume that each one of a given finite family I of counters is described by a bounded non-hermitian operator G_α ($\alpha \in I$). If only the counter α is present, the generator of the irreversible time evolution becomes $L_\alpha = H + G_\alpha$. Since G_α is bounded, this is well defined and we have $\operatorname{dom} L_\alpha = \operatorname{dom} H$. Each counter is further characterized by an exit space $\mathfrak{K}_\alpha$ with $j_\alpha : \operatorname{dom} L_\alpha \to \mathfrak{K}_\alpha$ and an exit observable F_α over a measurable space X_α. Following the general ideas described above we then define the generator L of the time evolution with all counters present as $L = H + \Sigma_\alpha G_\alpha$. The exit space of L can be taken as $\mathfrak{K} = \oplus_\alpha \mathfrak{K}_\alpha$ with $j : \operatorname{dom} L \to \mathfrak{K}$ defined as $j(\psi) = \oplus_\alpha j_\alpha(\psi)$. Since H is self-adjoint one readily verifies the equation

$$\begin{aligned}\langle j\psi, j\varphi \rangle &= \Sigma_\alpha \langle j_\alpha\psi, j_\alpha\varphi \rangle \\ &= \Sigma_\alpha \{ \langle iG_\alpha\psi, \varphi \rangle + \langle \psi, iG_\alpha\varphi \rangle \} = \langle iL\psi, \varphi \rangle + \langle \psi, iL\varphi \rangle .\end{aligned}$$

A natural exit observable F is defined on the disjoint union X of the spaces X_α such that for $\sigma \subset X_\alpha \subset X$ the operator $F(\sigma) \in \mathfrak{B}(\mathfrak{K})$ is equal to $F_\alpha(\sigma)$ on the summand $\mathfrak{K}_\alpha$ of $\mathfrak{K}$ and zero on all $\mathfrak{K}_\beta$ with $\beta \neq \alpha$.

Even if the time evolutions $\exp(-iL_\alpha t)$ are known, it is in general very difficult to compute the evolution $B_t = \exp(-iLt)$ and the exit time observable $\hat{F}$. This observable now contains a full description of the arrival probabilities at each counter, including the modifications of the arrival time distribution at counter α, which arise because particles captured at β never arrive at α, and also because particles may be scattered at β without being captured. These interactions between different counter sites become even stronger when we allow unbounded perturbations of the Hamiltonian. In the unbounded case there no longer is a general construction of the generator L in terms of H and the L_α. Nevertheless it is often clear how L must be defined. For example, if the generators H and L_α admit a common dense domain on which the closure of $L = H + \Sigma_\alpha(L_\alpha - H)$ is the generator of a contraction semigroup, then the above construction can be carried over with obvious modifications. A more singular case is given by the example of section II with a region whose boundary consists of several disconnected pieces α. The perturbation $G_\alpha = L_\alpha - H$ associated to each piece is then a complex « potential » with a δ-function singularity. Each of the generators L_α is well defined, but on $\cap_\alpha \operatorname{dom} L_\alpha$ each of these operators coincides with H. Hence $L = H \upharpoonright \cap_\alpha \operatorname{dom} L_\alpha$ is clearly not the generator of a semigroup. On the other hand L may be defined exactly as each of the L_α and the exit observable F measuring the arrival location on the boundary has a sum decomposition over the pieces α, which is exactly analogous to the above construction of F in terms of F_α.

An obvious difference between covariant time observables and the arrival time observables defined in section II is that the former assign an arrival time density to all times $t \in \mathbb{R}$, whereas the latter describe only arrival events with $t \geqslant 0$. The reason for this is that the semigroup B_t is defined only for $t \geqslant 0$, whereas the free evolution operators U_t are also defined for $t < 0$. It should be noted that this reversibility of U is not a necessary feature of the kinematical view of time evolution. As described in the introduction the operator U_t implements the operation of increasing the time between preparing and measuring by t seconds. For $t \geqslant 0$ this operation is usually easy to realize. For $t \leqslant 0$, however, this might mean that the measurement is to be carried out before the systems are prepared, which is clearly meaningless. Here one has to remember that different preparing procedures, which lead to the same expectation values for all observables are described by the same statistical state W. Thus the invertibility of the map $W \mapsto \mathfrak{U}_t(W) := U_t W U_t^*$ means that for any preparing procedure and any $t \geqslant 0$ we can find another preparation which becomes statistically indistinguishable from the given one after waiting for t seconds. The existence of the inverse $\mathfrak{U}_{-t}$ is not necessarily implied in the « kinematical » interpretation of $\mathfrak{U}_t$ as a waiting operation. In many applications, however, U_t is a one parameter subgroup of a larger symmetry group (Galilei or Poincaré group). The unitarity of U_t is then related to the stability of the particle under consideration. (Compare [*8*] for a description of unstable particles through representations of the Poincaré semigroup, in which only timelike forward translations are admitted). If U is unitary, as we shall assume from now on, and if we define $U_{-t} = U_t^*$, then an observable F over $\mathbb{R}^+$ satisfing the covariance condition $U_t^* F(\Theta) U_t = F(\Theta + t)$ for $t \geqslant 0$ and $\Theta \subset \mathbb{R}^+$ may immediately be extended to a covariant observable on the whole time axis.

Of course, reversible time evolutions may also be considered in the dynamical view of time evolution. In this case $W_t = \mathfrak{U}_t(W)$ is the state « at time t » for all times t under consideration (e. g. all times after the preparation of the system). The unitarity of the time evolution then means that given W_τ and some time $t < \tau$ there is a unique state W_t which will evolve into W_τ. We shall take this as a licence for calling also W_t the state of the system at time t. Suppose we want to perform a measurement on the system.

Then at some time τ we have bring the system in contact with a measuring device, thereby changing its time evolution from $\mathfrak{U}_t$ to a semigroup S_t. Hence the state of the system at time t will be $\mathfrak{U}_t W$ for $t \leqslant \tau$ and $S_{t-\tau}\mathfrak{U}_\tau W$ for $t \geqslant \tau$. Clearly, we can apply the formalism of section II to obtain for any exit observable F over X an arrival time observable $\hat{F}_\tau$ over $[\tau, \infty) \times X$. If $\tau \leqslant \rho$, $\sigma \subset X$, and $\Theta \subset [\rho, \infty)$ then $\hat{F}_\tau(\Theta \times \sigma)$ is defined as

$$\hat{F}_\tau(\Theta \times \sigma) = U_\tau^* \hat{F}((\Theta - \tau) \times \sigma) U_\tau = U_\tau^* B_{-\tau+\rho}^* \hat{F}((\Theta - \rho) \times \sigma) B_{\rho-\tau} U_\tau \qquad (8)$$

where $\hat{F}$ is the arrival time observable defined in section II and the second equality holds by covariance of $\hat{F}$ with respect to B_t. The index τ on $\hat{F}_\tau$ serves as a reminder that the probability tr $[W\hat{F}_\tau(\Theta \times \sigma)]$ for measuring an arrival in σ during the time interval Θ depends on the choice of τ. The physical reason for this is of course that the system might have interacted with the counter long before it was detected (e. g. by elastic scattering). However, we may expect that for systems approaching a fairly small counter from a large distance, these counting rates do not change very much if the counter is activated at earlier and earlier times. If it exists, we shall denote by $\hat{F}_\infty$ the weak limit $\hat{F}_\infty(\Theta \times \sigma) := \lim_{\tau \to -\infty} \hat{F}_\tau(\Theta \times \sigma)$. Note that since every bounded $\Theta \subset \mathbb{R}$ is eventually contained in an interval $[\tau, \infty)$ this defines an observable $\hat{F}_\infty$ over $\mathbb{R} \times X$. It is clear from eq. 8 that this limit exists if the strong limit $\Omega := \lim_{\tau \to -\infty} B_{-\tau} U_\tau$ exists on $\mathfrak{H}$. Then $\hat{F}_\infty(\Theta \times \sigma) = \Omega^* \hat{F}(\Theta \times \sigma)\Omega$ for $\Theta \subset \mathbb{R}^+$. Moreover, since $B_t\Omega = \Omega U_t$, $\hat{F}_\infty$ is a covariant observable with respect to the reversible time evolution U_t.

The existence of $\lim_{\tau \to \infty} B_\tau U_{-\tau}$ is sufficient but not necessary for the existence of $\hat{F}_\infty$. To see this consider the case of unitary B_t. Then $\mathfrak{K} = \{0\}$ and $\hat{F}_\tau \equiv 0 = \hat{F}_\infty$ for all τ, but the existence of the wave operator Ω depends on the details of B_t and U_t. In order to exclude this trivial case, let $\mathfrak{H}_0 = \{ \varphi \in \mathfrak{H} \mid \forall_{t>0} \| B_t\varphi \| = \| \varphi \| \}$ be the null space of J^*J as in section II, and let P denote the orthogonal projection onto $\mathfrak{H}_0^\perp$. Then P commutes with B_t [*9*, chapter 6.2] and $\hat{F}(\cdot) = \hat{F}(\cdot)P$ for all arrival time observables. Therefore, a more useful definition of the « wave operator » Ω in our case is

$$\Omega := \underset{\tau \to +\infty}{s\text{-lim}}\, PB_\tau U_{-\tau}. \qquad (9)$$

If this limit exists then indeed we have $\hat{F}_\infty(\Theta \times \sigma) = U_\rho^* \Omega^* \hat{F}((\Theta - \rho) \times \sigma)\Omega U_\rho$ for all $\sigma \subset X$ and $\Theta \subset [\rho, \infty)$, and $\hat{F}_\infty$ is covariant with respect to U_t. For some general results on the non-unitary scattering theory relevant for establishing the existence of this limit the reader is referred to [*10*] [*11*] [*12*].

Thus we may associate a covariant observable for the free time evolution with any counter or counter array whose interaction with the system is asymptotically negligible. A typical example in which this condition is violated is a system whose free evolution U_t has purely discrete spectrum

(e. g. a harmonic oscillator). In this case there are many bound states, so that even if the system « escapes absorption many times » it will stay close to the counter, so that there will be an appreciable probability for detection at a later time. In the limit $\tau \to -\infty$ the counter has been active for an infinite time and one may expect $\hat{F}_\infty = 0$. It is easy to prove this assertion under the assumption that Ω exists: since $\hat{F}_\infty$ is covariant with respect to U_t it must be supported by the absolutely continuous subspace of U_t [3, sect. 3] which is empty by assumption.

Like every covariant observable $\hat{F}_\infty$ admits a projection valued « dilation », i. e. there are a Hilbert space $\tilde{\mathfrak{H}}$, a unitary group $\tilde{U}_t$, a contraction $\tilde{J} : \mathfrak{H} \to \tilde{\mathfrak{H}}$ intertwining U_t and $\tilde{U}_t$, and a projection valued measure E in $\tilde{\mathfrak{H}}$ over $\mathbb{R} \times X$ such that $\hat{F}_\infty(\Theta \times \sigma) = \tilde{J}^* E(\Theta \times \sigma)\tilde{J}$ (see e. g. [3]). Assuming for simplicity that the exit observable F is projection valued, a dilation of $\hat{F}_\infty$ may easily be constructed as follows: we set $\tilde{\mathfrak{H}} = \mathfrak{L}^2(\mathbb{R}, dt; \mathfrak{K})$ with $(\tilde{U}_\tau\psi)(t) = \psi(t+\tau)$, and $E(\Theta \times \sigma) = G(\Theta) \otimes F(\sigma)$, where G denotes the multiplication by the characteristic function of $\Theta \subset \mathbb{R}$. Exactly like the operator J in section II the operator $(\tilde{J}\psi)(t) = j(\Omega U_t \psi)$ may be extended from dom H to all of $\mathfrak{H}$ and this extension is the required intertwining operator. The operator $\tilde{J}^*\tilde{J}$ describes the total response probability of the observable $\hat{F}_\infty$. Note that the space $\mathfrak{L}^2(\mathbb{R}^+, dt, \mathfrak{K})$ used in section II can be considered as a subspace of $\tilde{\mathfrak{H}}$ and that the projection of $\tilde{J}\psi$ into this subspace is equal to $J\Omega\psi$.

Since $\tilde{J}$ intertwines U_t and the shift $\tilde{U}_t$ it must vanish off the absolutely continuous subspace $\mathfrak{H}_{ac} \subset \mathfrak{H}$ of U_t. We may decompose $\mathfrak{H}_{ac} = \int^\oplus d\omega \mathfrak{H}_\omega$ such that U_t acts on each fiber $\mathfrak{H}_\omega$ like multiplication with $e^{-i\omega t}$. On the other hand $\tilde{\mathfrak{H}}$ may be identified by Fourier transformation with $\mathfrak{L}^2(\mathbb{R}, d\omega, \mathfrak{K}) \simeq \int^\oplus d\omega \mathfrak{K}$. By the intertwining property $\tilde{J}$ must admit a decomposition $\tilde{J} = \int^\oplus d\omega \tilde{J}(\omega)$ with $\tilde{J}(\omega) : \mathfrak{H}_\omega \to \mathfrak{K}$. Since $\tilde{J}$ is a contraction each $\tilde{J}(\omega)$ is a contraction. By definition of $\tilde{J}$ and inverse Fourier transformation we then have for $\psi \in \mathrm{dom}\, H$:

$$j\Omega\psi = (\tilde{J}\psi)(0) = (2\pi)^{-\frac{1}{2}} \int d\omega \tilde{J}(\omega)\psi(\omega). \tag{10}$$

This integral is well defined since $\| \tilde{J}(\omega) \|$ is uniformly bounded and $\| \psi(\omega) \|$ is integrable for $\psi \in \mathrm{dom}\, H$. This formula will be used below for calculating $\tilde{J}(\omega)$ from j and Ω. From $\tilde{J}(\cdot)$ the matrix elements of the observable $\hat{F}_\infty$ can be calculated as $\langle \varphi, \hat{F}_\infty(\Theta \times \sigma)\psi \rangle = \iint d\omega d\omega' \langle \varphi(\omega), K(\omega, \omega')\psi(\omega') \rangle$

with a kernel $K(\Theta, \sigma; \omega, \omega') : \mathfrak{H}_{\omega'} \to \mathfrak{H}_{\omega}$ given by

$$K(\Theta, \sigma; \omega, \omega') = \hat{\chi}_{\Theta}(\omega - \omega')\tilde{J}(\omega)^* F(\sigma)\tilde{J}(\omega') \tag{11}$$

where $\hat{\chi}_{\Theta}(\omega) := (2\pi)^{-1} \int_{t\in\Theta} dt e^{i\omega t}$ denotes the Fourier transform of the characteristic function of Θ. For the « time operator » $T = \int t\hat{F}_{\infty}(dt \times X)$, which describes the unnormalized expectation value of the arrival time, we formally obtain: $\langle \varphi, T\psi \rangle = \int d\omega \left\langle \tilde{J}(\omega)\varphi(\omega), \frac{1}{i}\frac{d}{d\omega} \tilde{J}(\omega)\varphi(\omega) \right\rangle$. Indeed, T is well defined on the domain of those ψ for which $\tilde{J}(\omega)\psi(\omega)$ has a square integrable derivative [*3*, sect. 3]. It is worth noting that the derivative of $\psi(\omega)$ alone makes no sense, since for $\omega \neq \omega'$ $\psi(\omega)$ and $\psi(\omega')$ lie in different spaces. Even if all fibers $\mathfrak{H}_{\omega}$ are identified with the same space $\mathfrak{H}_0$, the value of $\psi'(\omega)$ depends on the choice of this identification, i. e. ψ' changes under « gauge transformations » $\psi(\omega) \mapsto \Lambda(\omega)\psi(\omega)$ with unitary $\Lambda(\omega)$, whereas $\tilde{J}(\omega) \mapsto \tilde{J}(\omega)\Lambda(\omega)^*$ making the time operator T « gauge invariant ».

By covariance of $\hat{F}_{\infty}$ the observable $\sigma \mapsto \hat{F}_{\infty}(\mathbb{R} \times \sigma)$ commutes with U_t, hence can be measured together with the Hamiltonian. Explicitly, we can define an observable $\check{F}_{\infty}$ in $\mathfrak{H}_{ac}$ over $\mathbb{R} \times X$ by

$$\check{F}_{\infty}(\eta \times \sigma) = \int_{\omega\in\eta}^{\oplus} d\omega \tilde{J}(\omega)^* F(\sigma)\tilde{J}(\omega). \tag{12}$$

Then $\mathrm{tr}\,[W\check{F}_{\infty}(\eta \times \sigma)]$ is interpreted as the probability that the system has energy $\omega \in \eta$ and is detected at $x \in \sigma$ at some time $t \in \mathbb{R}$. Hence the arrival events $x \in X$ may not only measured together with the arrival time but also together with the energy of the free time evolution. In particular, $\tilde{J}(\omega)^* \tilde{J}(\omega) \in \mathfrak{B}(\mathfrak{H}_{\omega})$ is the operator describing the probability for a system of energy ω to be detected by $\hat{F}_{\infty}$.

Some typical features of this structure can be seen in the following example in which B_t, Ω, and $\tilde{J}(\omega)$ are evaluated explicitly.

IV. EXAMPLE

In this section we shall consider a particle on the half line $\mathbb{R}^+$ with inner degrees of freedom and its absorption at $x = 0$. The inner degrees of freedom will be described in a Hilbert space $\mathfrak{N}$ of dimension $n < \infty$, so that the Hilbert space of the whole system is $\mathfrak{H} = \mathfrak{L}^2(\mathbb{R}^+, dx; \mathfrak{N})$, the space of $\mathfrak{N}$ valued square integrable functions on $\mathbb{R}^+$. As in section II we shall take « absorption at the origin » to mean that the generator L of B_t is an extension of the symmetric operator $L_0\psi = -\frac{1}{2}\psi''$ defined on C^{∞} functions

$\psi : \mathbb{R}^+ \to \mathfrak{N}$, whose compact support does not contain $x = 0$. By using the isomorphism $\mathfrak{L}^2(\mathbb{R}, dx; \mathfrak{N}) \simeq \mathfrak{L}^2(\mathbb{R}^+, dx, \mathfrak{N} \oplus \mathfrak{N})$ all results of this section can be translated to the situation of a particle on the whole line with absorption at the origin.

The theory of the dissipative extensions L of a densely defined symmetric operator L_0 is almost identical with the standard theory [*13*] of symmetric and self adjoint extensions of L_0. This is due to the fact that as in the symmetric case a dissipative extension (i. e. an extension such that $\langle iL\psi, \psi \rangle + \langle \psi, iL\psi \rangle \geqslant 0$) is necessarily a restriction of the adjoint L_0^*. This follows by setting $\psi = \chi + \lambda\varphi$ in the above inequality with $\chi \in \operatorname{dom} L$, $\varphi \in \operatorname{dom} L_0$, and $\lambda \in \mathbb{R}$ large, and noting that the term quadratic in λ vanishes by symmetry of L_0. The operators between L_0 and L_0^* are in one-to-one correspondence with the subspaces of the quotient $\operatorname{dom} L_0^*/\operatorname{dom} L_0$. For the given operator L_0 the image of $\psi \in \operatorname{dom} L_0^*$ in this quotient is specified by the boundary values $\psi(0) \in \mathfrak{N}$ and $\psi'(0) \in \mathfrak{N}$. Then $\operatorname{dom} L_0^*/\operatorname{dom} L_0 \simeq \mathfrak{N} \oplus \mathfrak{N}$ carries a symmetric, but not positive, sesquilinear form $[\cdot, \cdot]$ given by

$$[\psi(0) \oplus \psi'(0), \varphi(0) \oplus \varphi'(0)] = \langle iL_0^*\psi, \varphi \rangle + \langle \psi, iL_0^*\varphi \rangle$$
$$= \frac{1}{2i}\{ \langle \psi'(0), \varphi(0) \rangle - \langle \psi(0), \varphi'(0) \rangle \}.$$

For $\varphi = \psi$ the expression is equal to $\mathcal{I}m \langle \psi'(0), \psi(0) \rangle$, i. e. the usual probability current across the boundary $x = 0$. The problem of finding contraction generators L extending L_0 thus reduces to finding maximal subspaces $\tilde{L} \subset \mathfrak{N} \oplus \mathfrak{N}$, on which the form $[\cdot, \cdot]$ is positive. The maximality of $\tilde{L}$ ensures that L is indeed a generator [*9*, theorem 6.4] and implies that $\dim \tilde{L} = \dim \mathfrak{N} = n$. The *exit space* $\mathfrak{K}$ of the resulting contraction semigroup is then equal to the space $\tilde{L}$ with inner product $[\cdot, \cdot]$ modulo the null space of this form.

The generator L is thus equal to the restriction of L_0^* to

$$\operatorname{dom} L = \{ \psi \in \operatorname{dom} L_0^* \mid A\psi(0) + B\psi'(0) = 0 \}$$

with suitable operators $A, B : \mathfrak{N} \to \mathfrak{N}$. For L to be a contraction generator, the map $\varphi_0 \oplus \varphi_1 \mapsto A\varphi_0 + B\varphi_1$ from $\mathfrak{N} \oplus \mathfrak{N}$ to $\mathfrak{N}$ has to be of rank n and $i(A^*B - B^*A)$ has to be positive (see eq. 15 below). Of course, the same boundary condition is specified by $A' = CA$, $B' = CB$ with a non singular matrix C. In particular, in the generic case of invertible B, we may set $C = B^{-1}$ so that we can choose $B' = \mathbb{1}$.

Our next task is to compute $B_t = \exp(-iLt)$. We could do this by applying Krein's resolvent formula, which yields $(L - z)^{-1}$ in terms of the resolvent of a fixed self adjoint extension of L_0. In the present case there is a more direct method, which generalizes the well known procedure for the Neumann (resp. Dirichlet) boundary condition $\psi'(0) = 0$ (resp. $\psi(0) = 0$). This procedure consists in identifying $\mathfrak{L}^2(\mathbb{R}^+, dx; \mathfrak{N})$ with the symmetric (resp. antisymmetric) subspace of $\mathfrak{L}^2(\mathbb{R}, dx; \mathfrak{N})$ with respect to reflection at the origin. Since the free evolution on $\mathbb{R}$ commutes with this reflection its restrictions to the (anti-)symmetric subspace is well defined and equal to the desired evolutions for Neumann and Dirichlet condition.

Let $\hat{\mathfrak{H}} = \mathfrak{L}^2(\mathbb{R}, dk; \mathfrak{N})$ and let $\hat{\mathrm{U}} = \exp(-i\hat{\mathrm{H}}t)$ with $(\hat{\mathrm{H}}\Phi)(k) = \frac{1}{2}k^2\Phi(k)$. In this space we define the involution Γ ($\Gamma^2 = \mathbb{1}$) by $(\Gamma\Phi)(k) = \Gamma(k)\Phi(-k)$, with

$$\Gamma(k) = (\mathrm{A} + ik\mathrm{B})^{-1}(\mathrm{A} - ik\mathrm{B}) \qquad (k \in \mathbb{R}). \tag{13}$$

We shall assume from now on that none of the finitely many poles of $\Gamma(z)$ in the complex plane lies on the real axis, so Γ is a bounded operator on $\hat{\mathfrak{H}}$. Note that $\Gamma(k)$ is unchanged if A and B are multiplied with an invertible matrix C, i. e. Γ depends on L but not on the matrices A, B chosen to represent the boundary conditions. Given a function $\Gamma(\cdot)$ which is regular at $\varkappa \in \mathbb{C}$ one obtains a possible choice of A and B by setting $\mathrm{A} = 1 + \Gamma(\varkappa)$ and $\mathrm{B} = (i\kappa)^{-1}(1 - \Gamma((\kappa))$. Inserting this into eq. 13 one sees that the admissable functions Γ are characterized by the condition

$$(k_1 - k_2)(\Gamma(k_1)\Gamma(k_2) - 1) = (k_1 + k_2)(\Gamma(k_1) - \Gamma(k_2)). \tag{14}$$

The Dirichlet and Neumann conditions correspond to $\mathrm{B} = 0$, $\Gamma(k) \equiv +1$ and $\mathrm{A} = 0$, $\Gamma(k) \equiv -1$, respectively. The function Γ is constant (hence satisfies $\Gamma(k)^2 = 1$), as in these two cases, iff the operator L scales under dilatations $x \mapsto \lambda x$ like the classical time evolution (i. e. $\mathrm{L} \mapsto \lambda^{-2}\mathrm{L}$). Otherwise the operator L will depend on some characteristic lengths. The above choice of A and B in terms of $\Gamma(\varkappa)$ shows that A and B can be taken to commute. Then it is clear that the space $\tilde{\mathrm{L}} \subset \mathfrak{N} \oplus \mathfrak{N}$ characterizing L consists of all vectors of the form $\mathrm{B}\varphi \oplus (-\mathrm{A}\varphi)$ for $\varphi \in \mathfrak{N}$. The dissipativity of L is hence equivalent to the positivity of $\mathcal{I}m < -\mathrm{A}\varphi, \mathrm{B}\varphi >$, i. e. $i(\mathrm{A}^*\mathrm{B} - \mathrm{B}^*\mathrm{A}) \geqslant 0$, which is equivalent to the positive definiteness of the kernel

$$(z_1, z_2) \mapsto (\bar{z}_1 + z_2)\{1 - \Gamma(z_1)^*\Gamma(z_2)\} + (\bar{z}_1 - z_2)\{\Gamma(z_1)^* - \Gamma(z_2)\}. \tag{15}$$

In particular, $1 - \Gamma(k)^*\Gamma(k)$ is positive for $k > 0$. Therefore each matrix element of $\Gamma(\cdot)$ is a rational function staying bounded at infinity so that $\Gamma(\infty)$ exists. By taking appropriate limits in eq. 14 and using $\|\Gamma(k)\| \leqslant 1$ for $k > 0$, we find that both operators $\Gamma(0)$ and $\Gamma(\infty)$ satisfy $\Gamma^2 = 1$ and $\Gamma^* = \Gamma$.

The connection between $\mathfrak{H}$ and $\hat{\mathfrak{H}}$ is given by the following operator $\mathrm{V} : \mathfrak{H} \to \hat{\mathfrak{H}}$ and its adjoint:

$$\begin{aligned} (\mathrm{V}\Psi)(k) &= (2\pi)^{-\frac{1}{2}} \int_0^\infty dx e^{-ikx}\Psi(x) \\ (\mathrm{V}^*\Phi)(x) &= (2\pi)^{-\frac{1}{2}} \int_{-\infty}^\infty dk e^{ikx}\Phi(k) \qquad (x \geqslant 0). \end{aligned} \tag{16}$$

Obviously $V^*V = \mathbb{1}$, and VV^* projects onto the space of functions, whose Fourier transforms have support in $\mathbb{R}^+$. The motivation for these definitions is that functions $V^*\Phi$ with $\Phi \in \operatorname{dom} \hat{H}$ and $\Phi + \Gamma\Phi = 0$ satisfy the boundary conditions:

$$\begin{aligned}
A(V^*\Phi)(0) + B(V^*\Phi)'(0) &= (2\pi)^{-\frac{1}{2}} \int dk(A + ikB)\Phi(k) \\
&= (2\pi)^{-\frac{1}{2}} \int dk(A - ikB)\Phi(-k) \\
&= (2\pi)^{-\frac{1}{2}} \int dk(A + ikB)(\Gamma\Phi)(k) \\
&= -(2\pi)^{-\frac{1}{2}} \int dk(A + ikB)\Phi(k) = 0 .
\end{aligned}$$

This leads to the following result:

PROPOSITION 5.1. — Let $\mathfrak{H}$, L, $\hat{\mathfrak{H}}$, $\hat{H}$, Γ and V be as above then:

(1) If $\Phi \in \operatorname{dom} \hat{H}$, $\Phi + \Gamma\Phi = 0$, then $V^*\Phi \in \operatorname{dom} L$ and
$$\exp(-itL)V^*\Phi = V^* \exp(-it\hat{H})\Phi .$$

(2) For $\Psi \in \operatorname{dom} L$, $(1 - \Gamma)V\Psi \in \operatorname{dom} \hat{H}$, and
$$\exp(-it\hat{H})(1 - \Gamma)V\Psi = (1 - \Gamma)V \exp(-itL)\Psi .$$

(3) $V^*\Gamma V\mathfrak{H} \subset \operatorname{dom} L$ and the operator $D_t = \exp(-itL)V^*\Gamma V$ is given by the integral kernel $D_t(x, y) = (2\pi)^{-1} \int_{\mathfrak{c}} dz \exp i\left(zx + zy - \frac{1}{2}z^2 t\right)\Gamma(z)$, where $\mathfrak{c}$ is a contour enclosing all poles of Γ in the upper half plane.

(4) $\exp(-itL) = V^* \exp(-it\hat{H})(1 - \Gamma)V + D_t$ for all $t \geqslant 0$.

(5) $V^*\Gamma V = D_0$ is the (non orthogonal) projection commuting with L onto the span of the pseudo-eigenvectors of L (i. e. the vectors annihilated by some non zero polynomial in L).

Proof. — (1) If $\Phi \in \operatorname{dom} H$, i. e. $k^2\Phi \in \mathfrak{L}^2(\mathbb{R})$, then Φ and $k\Phi$ are integrable because $(1 + |k|)^{-1} \in \mathfrak{L}^2(\mathbb{R})$. Hence the integrals in the above formal computation converge, showing that $V^*\Phi$ indeed satisfies the boundary conditions. If $\Phi \in \operatorname{dom} \hat{H}$, its Fourier transform has a square integrable distributional derivative on the whole axis, and in particular on $\mathbb{R}^+$. Hence $V^*\Phi \in \operatorname{dom} L$ and $LV^*\Phi = V^*\hat{H}\Phi$. By a straightforward computation using $(-k)^2 = k^2$ it is shown that Γ commutes with $\hat{H}$ so that the condition $\Phi + \Gamma\Phi = 0$ at time zero remains valid for $\Phi_t = \exp(-it\hat{H})\Phi$. The last relation thus follows by differentiation.

(2) By partial integration

$$(VL\Psi)(k) = \frac{1}{2}k^2(V\Psi)(k) + \frac{1}{2}(2\pi)^{-\frac{1}{2}}(\Psi'(0) + ik\Psi(0)) .$$

Since

$$(\Psi'(0)+ik\Psi(0))-\Gamma(k)(\Psi'(0)-ik\Psi(0))=(\mathrm{A}+ik\mathrm{B})^{-1}\cdot 2ik(\mathrm{A}\Psi(0)+\mathrm{B}\Psi'(0))=0,$$

we have $((1-\Gamma)\mathrm{VL}\Psi)(k)=\frac{1}{2}k^2((1-\Gamma)\mathrm{V}\Psi)(k)$, from which the claim follows easily.

(3) We show first that $\mathrm{V}^*\Gamma\mathrm{V}$ is given by the integral kernel $\mathrm{D}_0(x,y)$. Since this operator is bounded, it suffices to check this for matrix elements between vectors $\Psi_\nu\in\mathfrak{H}$ with $\Psi_\nu\in\mathfrak{L}^1(\mathbb{R}^+,dk;\mathfrak{N})$. Then

$$\langle \mathrm{V}\Psi_1,\Gamma\mathrm{V}\Psi_2\rangle = (2\pi)^{-1}\int dk\int dx_1\int dx_2 \exp ik(x_1+x_2)\langle \Psi_1(x_1),\Gamma(k)\Psi_2(x_2)\rangle .$$

Since $x_1, x_2 \geqslant 0$ and the integral converges absolutely, we may exchange the x- and k-integrations and close the path of the k-integration at infinity in the upper half plane, which proves the formula $\mathrm{V}^*\Gamma\mathrm{V}=\mathrm{D}_0$. For $\Psi\in\mathfrak{H}$ we have

$$\mathrm{A}(\mathrm{D}_t\Psi)(0)+\mathrm{B}(\mathrm{D}_t\Psi)'(0) = (2\pi)^{-1}\int dx\int_c dz \exp i\left(zx-\frac{1}{2}z^2t\right)(\mathrm{A}+iz\mathrm{B})\Gamma(z)\Psi(x)=0$$

since the integrand is analytic by definition of $\Gamma(z)$. Moreover,

$$-\frac{1}{2}(\mathrm{D}_t\Psi)''=\mathrm{LD}_t\Psi=i\frac{d}{dt}\mathrm{D}_t\Psi$$

is given by an absolutely convergent integral. Hence, $\mathrm{D}_t=\exp(-it\mathrm{L})\mathrm{V}\Gamma\mathrm{V}$ follows by integration.

(4) This is obvious from $\mathbb{1}=\mathrm{V}^*\mathrm{V}=\mathrm{V}^*((1-\Gamma)+\Gamma)\mathrm{V}$.

(5) Since $\exp(-it\mathrm{L})$ is a contraction semigroup

$$(\mathrm{L}-z)^{-1}=i\int_0^\infty dt\exp(-it\mathrm{L}+izt)$$

converges for $\mathscr{I}m\, z>0$ and the spectrum of L is contained in the closed lower half plane. Using the identity (4) we can split

$$(\mathrm{L}-z)^{-1}=\mathrm{V}^*(\hat{\mathrm{H}}-z)^{-1}(1-\Gamma)\mathrm{V}+\tilde{\mathrm{D}}_z,$$

where $\tilde{\mathrm{D}}_z$ is given by the kernel

$$\tilde{\mathrm{D}}_z(x,y)=(2\pi)^{-1}\int_c du\left(\frac{1}{2}u^2-z\right)^{-1}\exp iu(x+y)\Gamma(u).$$

The first term is analytic for $z\notin\mathbb{R}^+$ and comes from the absolutely continuous spectrum of L. The second term must contain the contributions of the pseudo-eigenvalues and the corresponding spectral projection is given according to the analytic functional calculus by $P = (-2\pi i)^{-1} \int dz\tilde{D}_z$. where the path of integration is a sufficiently large circle. Exchanging the integrations over z and u we obtain $P = D_0$. The rank of this projection is the number of poles of $\Gamma(z)$ for $\mathscr{I}m\, z > 0$ (counting multiplicities), hence less than $n = \dim \mathfrak{N} < \infty$. Consequently, $D_0\mathfrak{H}$ is spanned by the pseudo-eigenvectors of D_0LD_0. ■

Suppose now that the *free time evolution* in $\mathfrak{H}$ is given by a unitary group $U_t = \exp(-iHt)$, whose generator H is also an extension of L_0. We shall assume in addition that U_t scales under dilatations like the classical evolution so that the function $\Gamma(\cdot)$ characterizing H is of the form $\Gamma_0(k) \equiv R$, for some $R = R^*$ with $R^2 = 1$. Hence H satisfies Dirichlet conditions in one orthogonal subspace of $\mathfrak{N}$ and Neumann conditions in its complement.

Since the spectrum of U_t is purely absolutely continuous we may decompose $\mathfrak{H} = \mathfrak{H}_{ac} = \int^{\oplus} d\omega \mathfrak{H}_\omega$ as in the end of section III. Indeed, we may take $\mathfrak{H}_\omega \equiv \mathfrak{N}$ for all ω and define an isomorphism $I : \mathfrak{H} \to \int^{\oplus} d\omega \mathfrak{N} = \mathfrak{L}^2(\mathbb{R}^+, d\omega, \mathfrak{N})$ by

$$(I\psi)(\omega) = |2\omega|^{-1/4} \{ (V\psi)(\sqrt{2\omega}) - R \cdot (V\psi)(-\sqrt{2\omega}) \}$$

$$[(1 - \Gamma_0)VI^*\Phi](k) = \begin{cases} |k|^{\frac{1}{2}}\Phi\left(\frac{1}{2}k^2\right) & k > 0 \\ -|k|^{\frac{1}{2}}R\Phi\left(\frac{1}{2}k^2\right) & k < 0 \end{cases} \tag{17}$$

It is evident that the last operator intertwines multiplication by $e^{-\frac{1}{2}ik^2t}$ in $\hat{\mathfrak{H}}$ and multiplication by $e^{-i\omega t}$ in $\mathfrak{L}^2(\mathbb{R}^+, d\omega, \mathfrak{N})$. Hence I intertwines $e^{-i\omega t}$ and $U_t = V^* \exp(-iHt)(1 - \Gamma_0)V$.

We now want to calculate the *wave operator* Ω from eq. 9. It is easy to see that $PD_t \to 0$ in operator norm as $t \to \infty$. For this we split D_t into contributions from poles of $\Gamma(z)$ with $\mathscr{R}e\, z < 0$ and $\mathscr{R}e\, z = 0$ respectively (other possibilities are excluded since L is dissipative). The first kind of contribution vanishes like

$$\left|\exp\left(-\frac{1}{2}iz^2t\right)\right| = \exp\left(\frac{1}{2}t\,\mathscr{I}m\, z^2\right) = \exp(t\,\mathscr{I}m\, z \cdot \mathscr{R}e\, z).$$

Vectors Φ in the image of a contribution of the second kind satisfy $\exp(-itL)\Phi = \mathfrak{P}(t)\exp(i\lambda t)\Phi$ for some polynomial $\mathfrak{P}$ and $\lambda \in \mathbb{R}$. Since $\exp(-itL)$ is a contraction $\mathfrak{P}$ has to be constant, hence Φ is in the unitary subspace of B_t and $P\Phi = 0$ by definition of P. Hence only the first term in the decomposition (4) of proposition 5.1 remains and

$$\Omega = \underset{t \to +\infty}{s\text{-lim}}\, PV^*(1 - \Gamma)\exp(-i\hat{H}t)VV^*\exp(i\hat{H}t)(1 - \Gamma_0)V . \tag{18}$$

This limit is computed by using the following lemma, which is a one dimensional version of « scattering into cones » [14]. Put in terms of classical mechanics it says that for a free particle on $\mathbb{R}$ $x_t \to +\infty$ in position space as $t \to -\infty$ is equivalent to $k < 0$ in momentum space.

LEMMA 5.2. — Let $\hat{\mathfrak{H}}$, $\hat{U}_t$, $\mathfrak{H}$, and V be as above and let $\Xi \in \mathfrak{B}(\hat{\mathfrak{H}})$ denote the operator of multiplication with the characteristic function of $\{ k \mid k \leqslant 0 \}$. Then

$$\underset{t \to +\infty}{s\text{-lim}} \exp(-i\hat{H}t)VV^*\exp(+i\hat{H}t) = \Xi . \tag{19}$$

Hence the limit in eq. 18 exists and is equal to

$$\Omega = PV^*(1 - \Gamma)\Xi(1 - \Gamma_0)V = P\tilde{\Omega} .$$

For the application of eq. 10 we need $j\Omega = j\tilde{\Omega} : \mathrm{dom}\, H \to \mathfrak{K}$, written in energy representation, i. e. $j\tilde{\Omega}I^*$. Recall that $\mathfrak{K}$ was defined as a subspace of $\mathfrak{N} \oplus \mathfrak{N}$, the space of boundary values at $x = 0$. A straightforward calculation combining this result with eq. 17 now yields

$$\begin{aligned} (\tilde{\Omega}I^*\Phi)(0) &= (2\pi)^{-\frac{1}{2}} \int_0^\infty d\omega\, |2\omega|^{-1/4} i(-1 + \Gamma(-\sqrt{2\omega}))R\Phi(\omega) \\ (\tilde{\Omega}I^*\Phi)'(0) &= (2\pi)^{-\frac{1}{2}} \int_0^\infty d\omega\, |2\omega|^{+1/4} i(1 + \Gamma(-\sqrt{2\omega}))R\Phi(\omega) . \end{aligned} \tag{20}$$

Comparing this with eq. 10 we obtain for $\tilde{J}(\omega) : \mathfrak{N} \to \mathfrak{K} \subset \mathfrak{N} \oplus \mathfrak{N}$:

$$\tilde{J}(\omega) = \{ |2\omega|^{-1/4}(-1+\Gamma(-\sqrt{2\omega}))R \} \oplus \{ |2\omega|^{+1/4} i(1+\Gamma(-\sqrt{2\omega}))R \} . \tag{21}$$

Setting $\tilde{J}(\omega) = \alpha \oplus \beta$ we find the absorption probability $\tilde{J}(\omega)^*\tilde{J}(\omega) \in \mathfrak{B}(\mathfrak{N})$ at energy ω from

$$\langle \tilde{J}(\omega)\varphi, \tilde{J}(\omega)\psi \rangle_{\mathfrak{K}} = [\alpha\varphi \oplus \beta\varphi, \alpha\psi \oplus \beta\psi] = \frac{1}{2i} \langle \varphi, (\beta^*\alpha - \alpha^*\beta)\psi \rangle :$$

$$Q(\omega) := \tilde{J}(\omega)^*\tilde{J}(\omega) = R^* \{ 1 - \Gamma(\sqrt{2\omega})^*\Gamma(-\sqrt{2\omega}) \} R . \tag{22}$$

By the discussion after eq. 15 we have $0 \leqslant Q(\omega) \leqslant 1$. Since we have assumed $\Gamma(\cdot)$ to be non singular on the real axis there is even a constant $p < 1$ such that $Q(\omega) \leqslant p1$. Moreover $Q(0) = Q(\infty) = 0$, so there is no absorption for very high and very low energies. Unless Q vanishes identically these are the only zeros of Q: if $\Gamma(k)^*\Gamma(k) = 1$ for some $k \in \mathbb{R}$, then $B^*A - A^*B = 0$ which means that L is self-adjoint.

By a similar computation one obtains the « time operator » $T = \int t\hat{F}_\infty(dt \times X)$:

$$(T\psi)(\omega) = Q(\omega)\frac{1}{i}\frac{d\psi}{d\omega} + \frac{1}{2i}\frac{dQ}{d\omega}\psi(\omega) + \tilde{T}(\omega)\psi(\omega) \tag{23}$$

with $$\tilde{T}(\omega) = \frac{i}{8\omega}\{\Gamma(\sqrt{2\omega})^{*2} - \Gamma(\sqrt{2\omega})^2\}.$$

The special case of this example with $\dim \mathfrak{N} = 1$ is also a special case of the example in section II, where $A = a$, $B = 1$. Then dissipativity of L requires $\mathscr{I}m\, a \geqslant 0$, and the technical requirement that $\Gamma(z) = (a+iz)^{-1}(a-iz)$ has no poles with $z \in \mathbb{R}$ means that $\mathscr{R}e\, a \neq 0$. Taking the Dirichlet boundary condition $R = 1$ for the free evolution we obtain:

$$Q(\omega) = \frac{4\sqrt{2\omega}\,\mathscr{I}m(a)}{|a + i\sqrt{2\omega}|^2}; \qquad \tilde{T}(\omega) = -\frac{\sqrt{2}\,\mathscr{R}e(a)(a^2 - 2\omega)}{\sqrt{\omega}\,|a + i\sqrt{2\omega}|^4}. \tag{24}$$

These results about $\hat{F}_\infty$ are to be compared with the « ideal » covariant time observable F_c in the sense of [3]. One obtains such observables by postulating as many properties as possible known for the classical observable « time of arrival at the origin ». As a covariant observable F_c is characterized by a family $J_c(\omega): \mathfrak{N} \to \mathfrak{K}_c$ of contractions, where $\mathfrak{K}_c$ is some auxiliary Hilbert space. The first condition one requires of an ideal covariant observable is that every particle is detected, i. e. $J_c(\omega)^*J_c(\omega) = 1$. Since we have demanded classical scaling behaviour ($x \mapsto \lambda x$, $k \mapsto \lambda^{-1}k, \omega \mapsto \lambda^2\omega$) of the free time evolution, it is natural to require this scaling behaviour also of the observable F_c (i. e. $t \mapsto \lambda^{-2}t$). This is equivalent to postulating that $J_c(\omega) \equiv J_c$ is a constant isometry. We may thus identify $\mathfrak{K}_c$ with $\mathfrak{N}$ and take J_c as the identity. The corresponding time operator is simply $T_c = -i\dfrac{d}{d\omega}$. (Note that in spite of the remarks in section III, the differentiation of ψ makes sense here, since the dilatation group induces a canonical identification of the spaces $\mathfrak{H}_\omega$).

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REFERENCES

[1] G. LUDWIG, *Foundation of quantum mechanics* (2 vol.), Springer, Berlin, 1983 and 1985.

[2] E. B. DAVIES, *Quantum theory of open systems*. Academic, London, 1976.

[3] R. WERNER, « Screen Observables in relativistic and nonrelativistic quantum mechanics ». *J. Math. Phys.*, t. **27**, 1986, p. 793-803.

[4] E. B. DAVIES, Non-unitary scattering and capture. Part I: Quantum dynamical semigroup theory. *Ann. Inst. H. Poincaré*, t. **32 A**, 1980, p. 361-375.

[5] R. HAAG, D. KASTLER, An algebraic approach to quantum field theory. *J. Math. Phys.*, t. **5**, 1964, p. 848-861.

[6] K.-E. HELLWIG, K. KRAUS, Formal description of measurements in local quantum field theory. *Phys. Rev.*, t. **D 1**, 1970, p. 566-571.

[7] R. WERNER, Local preparability and the split property in quantum field theory. *Lett. Math. Phys.*, t. **13**, 1987, p. 325-329.

[8] R. ALICKI, M. FANNES, A. VERBEURE, *Unstable particles and the Poincaré semigroup in quantum field theory*. Preprint, Leuven, 1985.

[9] E. B. DAVIES, *One-parameter semigroups*. Academic, London, 1980.

[10] Ph. A. MARTIN, Scattering theory with dissipative interactions and time delay. *Nuovo Cim.*, t. **30 B**, 1975, p. 217-238.

[11] E. B. DAVIES, Non-unitary scattering and capture. Part I: Hilbert space theory. *Commun. Math. Phys.*, t. **71**, 1980, p. 277-288.

[12] H. NEIDHART, *A dissipative scattering theory*. In: H. Helson, B. Sz. Nagy, F.-H. Vasilescu, D. Voiculescu (eds.): « Spectral theory of linear operators and related topics », Birkhäuser, Basel, 1984.

[13] N. I. ACHIEZER, I. M. GLAZMAN, *Theory of linear operators in Hilbert space*, vol. 2, Pitman, London, 1981.

[14] J. M. JAUCH, R. LAVINE, R. G. NEWTON, Scattering into cones. *Helv. Phys. Acta*, t. **45**, 1972, p. 325-330.

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