Semi-Groups and Time Operators for Quantum Unstable Systems

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We use spectral projections of time operator in the Liouville space for simple quantum scattering systems in order to define a space of unstable particle states evolving under a contractive semi-group. This space includes purely exponentially decaying states that correspond to complex eigenvalues of this semi-group. The construction provides a probabilistic interpretation of the resonant states characterized in terms of the Hardy class.

KEY WORDS: quantum ustable system; time operator; semigroup time evolution; Hardy spaces; Liouville spaces.

1. INTRODUCTION

We shall consider the unstable particle states of a quantum mechanical system in the framework of the Liouville von-Neumann time evolution. The decay processes are generally described by exponential time distributions with a given characteristic "lifetime." As well known, such properties are unattainable within the standard quantum mechanics on account of deviation from the exponential decay (see Chiu *et al.*, 1977; Horwitz and Marchand, 1971; Misra and Sudarshan, 1977 and references therein to previous works). Several attempts have been proposed to overcome these difficulties and it was proposed to obtain these phenomena as resulting from semi-group evolutions (Bohm and Gadella, 1989; Horwitz and Marchand, 1971). For example, It has been suggested by Horwitz and Marchand (1971) to describe the decaying system by a subspace $P\mathfrak{H}$ of $\mathfrak{H}$ such that the family $Pe^{-itH}P$ can be approximated by a semi-group of contractive operators, where P is some orthogonal projection. The semi-group is associated to poles of the reduced resolvent $P\frac{1}{H-z}P$ and the unstable space is generally defined

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according to Weisskopf–Wigner theory. That is, briefly speaking, the Hamiltonian is represented as a sum of a free Hamiltonian H_0 and some interaction potential gV, where g is a coupling constant:

$$H = H_0 + gV \tag{1.1}$$

and the subspace $P\mathfrak{H}$ is taken as the space of eigenvectors of H_0 expected to decay under the total evolution group e^{-itH}. In that case, the decay law of the unstable particles, which expresses the probability that the unstable states $\phi \in P\mathfrak{H}$, created at time $t = 0$, is still in the subspace $P\mathfrak{H}$ at time t, is given by:

$$p_\phi(t) = \|Pe^{-itH}\phi\|^2 \tag{1.2}$$

However, the semi-group property does not hold and the family $Pe^{-itH}P$ only obeys to a generalized Master Equation deviating from the pure exponential decay on account of essential singularities of the reduced resolvent (see e.g. Courbage, 1982a,b; Horwitz and Marchand, 1971 for a treatment of this aspect in the Liouville space).

In this paper we study a semi-group evolution obtained from time operators introduced in the Liouville space formulation of quantum mechanics in Misra *et al.* (1979) and whose existence and construction given in Courbage (1980).

To start with a brief recapitulation, let H be the Hamiltonian of the system acting on the Hilbert space $\mathfrak{H}$. The "Liouville space," denoted $\mathfrak{L}$, is the space of Hilbert–Schmidt operators ρ on $\mathfrak{H}$ such that $Tr(\rho^*\rho) < \infty$, equipped with the scalar product: $\langle \rho, \rho' \rangle = Tr(\rho^*\rho')$. The time evolution of these operators is given by the Liouville von-Neumann group of operators:

$$U_t\rho = e^{-itH}\rho e^{itH} \tag{1.3}$$

The infinitesimal self-adjoint generator of this group is the Liouville von-Neumann operator L given by:

$$L\rho = H\rho - \rho H \tag{1.4}$$

That is, $U_t = e^{-itL}$. Some more mathematical details on this operator may be found, e.g., in Courbage (1982a,b).

Here, instead of the evolution group e^{-itH} on $\mathfrak{H}$ we shall consider the group e^{-itL} on $\mathfrak{L}$ and we shall use as a projection operator P on the subspace of unstable states the one associated to spectral decomposition of time operator as will be explained in Sec. 2.

It is well-known Jammer (1974) that tentative constructions of a time operator for quantum mechanical systems leading to a rigorous understanding of the fourth uncertainty relation faced the remark of Pauli concerning the nonexistence of a

canonically conjugated operator T to the time evolution generator H, verifying:

$$[H, T] = i I$$

on account of the lower semiboundedness of the spectrum of the Hamiltonian. However, time operator was considered in the framework of the Liouville von-Neumann space and the fourth uncertainty relation has been derived through it (Courbage, 1980). Here we shall restrict to this framework. In Sec. 3, we give a mathematical characterization of the subspace of unstable states which has the structure of the Lax-Phillips theory (Lax and Phillips, 1967).

2. UNSTABLE STATES AND TIME OPERATORS IN THE HILBERT-SCHMIDT SPACE

A sufficient condition for the existence of a self-adjoint time operator canonically conjugated to the Liouville operator, i.e.:

$$[L, T] = -i I \qquad (2.1)$$

is that the Hamiltonian has unbounded and lower semi-bounded (absolutely) continuous spectrum. We shall suppose that H has no singular discrete or continuous spectrum. In the opposite case, T should be defined on the orthogonal of this singular subspace. The construction is recapitulated in the next section. Equation 2.1 is equivalent to the Weyl relation:

$$U_{-t} T U_t = T + t I \qquad (2.2)$$

Denoting by P_τ the family of spectral projection operators of T defined by:

$$T = \int_{\mathbb{R}} \tau \, d P_\tau$$

we have the following properties:

  i) $P_\tau P_{\tau'} = P_\tau$ if $\tau \leq \tau'$ (a characteristic property of any spectral projection operators family)
  ii) $U_t P_\tau U_{-t} = P_{\tau+t}$ (an equivalent property of the Weyl relation).

It defines the family of subspaces $\mathcal{F}_\tau$, on which projects P_τ, verifying:

  i)' $\mathcal{F}_\tau \subseteq \mathcal{F}_{\tau+t}$ for $t \geq O$
  ii)' $U_t \mathcal{F}_\tau = \mathcal{F}_{\tau+t}$.

As proposed in Courbage (1987, 2001), we associate the subspace $\mathcal{F}_{t_0}$ to the set of decaying initial states prepared at time t_0. Shifting the origin of time to the "time of preparation" t_0 allows to consider, without loss of generality, P_0 as a projection operator on the subspace of the unstable states.

In fact, two important properties are fulfilled by this subspace which enable it to realize such description.

First, it was proved that time operator satisfies to the fourth uncertainty relation between time and energy (Courbage, 1980) with the following sense. Considering that a time operator should be a quantum observable, like spatial position and energy, which describes the time occurrence of specified events such as time of arrival of a beam of particles to a screen or time of decay of unstable particles and extending the von-Neumann formulation of quantum mechanics to Liouville space, it is possible to define the states of a quantum system by normalized elements $\rho \in \mathfrak{L}$ with respect to the scalar product, the expectation of T in the state ρ by:

$$\langle T \rangle_\rho = \langle \rho, T\rho \rangle \tag{2.3}$$

and the "uncertainty" of the observable T as its fluctuation in the state ρ:

$$(\Delta T)_\rho = \sqrt{\langle T^2 \rangle_\rho - (\langle T \rangle_\rho)^2} \tag{2.4}$$

Embedding the normalized elements $\psi \in \mathfrak{H}$ as elements $\rho = |\psi\rangle\langle\psi| \in \mathfrak{L}$, and the observables A operating on $\mathfrak{H}$ as observables $\hat{A}$ operating on $\mathfrak{L}$ as a multiplication by A: $\hat{A}\rho = A.\rho$, the above definition coincides with the usual quantum rule giving the expectation of an observable A, operating on $\mathfrak{H}$, in the state $\psi \in \mathfrak{H}$:

$$\langle A \rangle_\rho = \langle \rho, \hat{A}\rho \rangle = \langle \psi, A\psi \rangle \tag{2.5}$$

A density matrix state M (i.e., a positive operator on $\mathfrak{H}$ with $Tr(M) = 1$), is embedded in $\mathfrak{L}$ as element $\rho = M^{1/2}$. Then, the expectation of the observable A operating on $\mathfrak{H}$ in the mixture state M usually given by $Tr(M.A)$ is also preserved, for:

$$\langle A \rangle_\rho = \langle \rho, \hat{A}\rho \rangle = Tr(M.A) \tag{2.6}$$

Let ΔE be the usual energy uncertainty in the state M given by:

$$\Delta E = \sqrt{Tr(MH^2) - (Tr(M.H))^2} \tag{2.7}$$

and $\Delta T = (\Delta T)_{M^{1/2}}$ be the uncertainty of T in the state M defined as in (2.4). It has been shown that:

$$\Delta E.\Delta T \geq \frac{1}{2\sqrt{2}} \tag{2.8}$$

This uncertainty relation leads to the interpretation of T as the time occurrence of specified random events. The time of occurrence of such events fluctuates and we speak of the probability of its occurrence in a time interval $I =]t_1, t_2]$. The observable T' associated to such event in the initial state ρ_0 has to be related to

the time parameter t by:

$$\langle T' \rangle_{\rho_t} = \langle T' \rangle_{\rho_0} - t \tag{2.9}$$

where $\rho_t = e^{-itL}\rho_0$. Comparing this condition with the above Weyl relation we see that we have to define T' as: $T' = -T$. Let P'_τ be the family of spectral projections of T', then, in the state ρ, the probability of occurrence of the event in a time interval I is given, as in the usual von Neumann formulation, by:

$$P(I, \rho) = \|P'_{t_2}\rho\|^2 - \|P'_{t_1}\rho\|^2 = \|(P'_{t_2} - P'_{t_1})\rho\|^2 := \|P'(I)\rho\|^2 \tag{2.10}$$

The unstable "undecayed" states prepared at $t_0 = 0$ are the states ρ such that $P(I, \rho) = 0$ for any negative time interval I, that is:

$$\|P'_\tau\rho\|^2 = 0, \forall \tau \le 0 \tag{2.11}$$

In other words, these are the states verifying $P'_0\rho = 0$. It is straightforwardly checked that the spectral projections P'_τ are related to the spectral projections P_τ by the following relation:

$$P'_\tau = 1 - P_{-\tau} \tag{2.12}$$

Thus, the unstable states are those states verifying: $\rho = P_0\rho$ and they coincide with our subspace $\mathcal{F}_0$. For these states, the probability that a system prepared in the undecayed state ρ is found to decay sometime during the interval $I = \,]0, t]$ is $\|P'_t\rho\|^2 = 1 - \|P_{-t}\rho\|^2$, a monotonically nondecreasing quantity which converges to 1 as $t \to \infty$ for $\|P_{-t}\rho\|^2$ tends monotonically to zero. As noticed by Misra and Sudarshan (1977), such quantity could not exist in the usual quantum mechanical treatment of the decay processes and could not be related to the "survival probability" (1.2) for it is not a monotonically decreasing quantity in the Hilbert space formulation. In the Liouville space, given any initial state ρ, its survival probability in the unstable space is given by:

$$p_\rho(t) = \|P_0 e^{-itL}\rho\|^2 \tag{2.13}$$

This survival probability and the probability of finding the system to decay sometime during the interval $I = \,]0, t]$, are related by:

$$\|P'_t\rho\|^2 = 1 - \|P_{-t}\rho\|^2$$
$$= 1 - \|U_{-t}P_0 U_t\rho\|^2$$
$$= 1 - \|P_0 e^{-itL}\rho\|^2$$
$$= 1 - p_\rho(t) \tag{2.14}$$

The survival probability is monotonically decreasing to 0 as $t \to \infty$. This is true for for any general initial state as it can be seen from the Eq. 2.14. It should be

noted that the projection operator P_0 is not a "factorizable" operator, that is, not of the form $P_0\rho = E\rho E$ where E is a projection operator in $\mathfrak{H}$.

Second, for any time preparation t_0, the projection $P_{t_0}\rho_t$ obeys to a closed equation (i.e., it depends only on the projected initial condition $P_{t_0}\rho(0)$) given by a contraction semi-group for $t > t_0$. This is a consequence of the properties i) and ii) leading for any $t > t_0$ to:

$$P_{t_0} = P_{t_0} P_{t_0+t} = P_{t_0} U_t P_{t_0} U_{-t}$$

Thus, multiplying both members by U_t, we obtain:

$$P_{t_0} U_t = P_{t_0} U_t P_{t_0} \tag{2.15}$$

It implies that the one parameter family of operators:

$$W_t = P_{t_0} U_t = P_{t_0} U_t P_{t_0} \tag{2.16}$$

is a semi-group for $t > t_0$:

$$W_t W_{t'} = W_{t+t'} \tag{2.17}$$

for any $t, t' > t_0$. It is also evident that this is a contractive semi-group, i.e., $\|W_t\| \leq 1$, with respect to the operator norm on $\mathfrak{L}$. Note that Eq. 2.15 is nothing but the fact that the space $\mathcal{F}_{t_0}^{\perp}$, orthogonal to $\mathcal{F}_{t_0}$, is invariant under U_{-t}.

The above semi-group has quite analog structure than the Lax-Phillips semi-group (Lax and Phillips, 1967). For more informations on the applications of this structure, we refer to the paper of Y. Strauss (2003) and references therein.

3. MATHEMATICAL CHARACTERIZATION OF P_0 AND W_t

In this section, we shall restrict to the case where the Hamiltonian H has a simple Lebesgue spectrum extending from 0 to $+\infty$. Some models, like Friedrichs models (1948), verify this assumption which is useful in order to illustrate the description of unstable states in the Hilbert-Schmidt space.

Choosing a spectral representation of H, any $\psi \in \mathfrak{H}$ is represented by a square integrable function $\psi(\lambda) \in L^2(\mathbb{R}^+)$ and the Hamiltonian is represented by the multiplication operator by λ, that is, $H\psi(\lambda) = \lambda\psi(\lambda)$. The Hilbert-Schmidt operators on $L^2(\mathbb{R}^+)$ are the integral operators associated to square-integrable kernels, $\rho(\lambda, \lambda') \in L^2(\mathbb{R}^+ \times \mathbb{R}^+)$. The Liouville operator is given by: $L\rho(\lambda, \lambda') = (\lambda - \lambda')\rho(\lambda, \lambda')$. Now the spectral representation of L is obtained through the change of variables: $(\lambda, \lambda') \to (\nu, E)$ defined by:

$$\nu = \lambda - \lambda' \tag{3.1}$$

$$E = \min(\lambda, \lambda') \tag{3.2}$$

In the spectral representation of L, we denote again, for the sake of simplicity, a Hilbert-Schmidt operator on $\mathfrak{H}$ by $\rho(v, E) \in L^2(\mathbb{R} \times \mathbb{R}^+)$, thus:

$$L\rho(v, E) = v\rho(v, E) \tag{3.3}$$

Time operator $T\rho(v, E)$ is then the self-adjoint extension of the operator $i\frac{\partial}{\partial v}\rho(v, E)$. Under this hypothesis on the Hamilton operator we obtain a spectral representation of T using the Fourier Transform

$$\hat{\rho}(\tau, E) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{i\tau v} \rho(v, E) \, dv$$

In this representation, the time operator will be given by: $T\hat{\rho}(\tau, E) = \tau\hat{\rho}(\tau, E)$ and the spectral projection operator P_τ is the multiplication operator by the characteristic function of $] - \infty, \tau]$ denoted $\chi_{]-\infty,\tau]}$. It follows from the Paley–Wiener theorem that the subspace of unstable states $\mathcal{F}_0$ is characterized as the boundary values on $\mathbb{R}$ of the upper Hardy class of complex functions $\mathfrak{H}^+$ defined as the functions $\rho(z, E)$ that are upper-plane analytic vector valued of $z \in \mathbb{C}_+ = \{z \in \mathbb{C} : Im(z) > 0\}$ such that:

$$\sup_{y>0} \int_{-\infty}^{+\infty} \|\rho(x + iy, E)\|_E dy < \infty \tag{3.4}$$

where $\|\rho(x + iy, E)\|_E^2 = \int_0^{+\infty} |\rho(x + iy, E)|^2 dE$. It is also clear that the complementary orthogonal projection operator is the multiplication operator by the characteristic function of $]0, +\infty[$ on the space of the boundary values on $\mathbb{R}$ of the lower Hardy class $\mathfrak{H}^-$. It follows that a state $\rho(v, E) \in L^2(\mathbb{R} \times \mathbb{R}^+)$ belongs to $\mathcal{F}_0$ if and only if $\rho(v, E)$ belongs to the Hardy space $\mathfrak{H}^+$. As $\mathfrak{L} = \mathfrak{H}^+ \oplus \mathfrak{H}^-$, any initial state ρ is decomposed into a sum $\rho = \rho^+ + \rho^-$ of unstable component $\rho^+ \in \mathfrak{H}^+$ and some orthogonal component $\rho^- \in \mathfrak{H}^-$.

Let us note that we used a slight generalization of the Paley-Wiener theorem. The original theorem was formulated in $L^2(\mathbb{R})$. But we can reduce the space $L^2(\mathbb{R} \times \mathbb{R}^+)$ to a countable direct sum of copies of $L^2(\mathbb{R})$, by taking a basis $\phi_k(E)$ of $L^2(\mathbb{R}^+)$ and expanding $\rho(v, E)$ on this basis: $\rho(v, E) = \sum_{k=0}^{\infty} a_k(v)\phi_k(E), a_k(v) \in L^2(\mathbb{R})$. Any $\rho(v, E) \in L^2(\mathbb{R} \times \mathbb{R}^+)$ is then identified with the corresponding sequence of functions $\{a_k(v)\}$, for each of its elements the Paley-Wiener theorem applies. The same argument should be understood in what follows.

For a general state the decay rate of the survival probability is not exponential. However, there is a family of unstable initial states whose evolution under the semi-group W_t has purely exponential decay:

Theorem 3.1.   For any $\xi \in \mathbb{C}_- = \{z \in \mathbb{C} : Im(z) < 0\}$, $e^{-it\xi}$ is an eigenvalue of the semi-group W_t corresponding to the eigenfunctions:

$$\rho_\xi(\nu, E) = \frac{\psi(E)}{\nu - \xi}, \quad \psi \in L^2(\mathbb{R}^+) \tag{3.5}$$

.

Proof: The function $\rho_0(\nu, E) = \frac{\psi(E)}{\nu - \xi}, \in \mathfrak{H}^+$, so that $\rho_0 = P_0 \rho_0$. Thus, in the spectral representation of L, $\rho_t(\nu, E) := U_t \rho_0(\nu, E) = \frac{e^{-it\nu} \psi(E)}{\nu - \xi}$, and denoting by $\hat{\rho}_t(\tau, E) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{i\tau\nu} \rho_t(\nu, E)$ the Fourier transform of ρ_t with respect to ν, we obtain for $\tau < 0$ and $t > 0$, $P_0 \hat{\rho}_t(\tau, E) = \hat{\rho}_t(\tau, E) = -\sqrt{2\pi} i e^{i(\tau - t)\xi} \psi(E)$, and $P_0 \hat{\rho}_t(\tau, E) = 0$ for $\tau > 0$. Taking the inverse Fourier transform of $P_0 \hat{\rho}_t(\tau, E)$ we obtain in the spectral representation of the Liouville operator:

$$W_t \rho_0(\nu, E) = P_0 U_t \rho_0(\nu, E) = \frac{e^{-it\xi} \psi(E)}{\nu - \xi} \tag{3.6}$$

for $t > 0$. $\square$

It follows that these states have purely exponentially decaying survival probability. It is also a result of the Eq. 2.16 and the above theorem that initial states with unstable part of the form (3.5) will also have purely exponentially decaying survival probability.

4. SOME CONCLUDING REMARKS

The semi-group derived from time operator is analog to the semi-group derived from Lax-Phillips evolution. Thus, Liouville space provides a natural realization of the Lax-Phillips structure and a definition of the resonances states. The above eigenfunctions of W_t are the analog of the Gamow states much studied recently in the frame of rigged Hilbert space (Bohm and Gadella, 1989). But, the introduction of a time operator allows to give them a probabilistic content.

We shall apply the above construction in a forthcoming paper to some simple scattering models extended in the Liouville space, like the Friedrichs model. Recently, the expectation of time operator in the free Hamiltonian eigenfunctions state of this model has been computed and it has been shown that it coincides with the lifetime of the resonance (Ordoñez *et al.*, 2001).

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