On the existence of Lyapounov variables for Schrödinger evolution

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Abstract

The theory of (classical and) quantum mechanical microscopic irreversibility developed by B. Misra, I. Prigogine and M. Courbage (MPC) and various other contributors is based on the central notion of a Lyapounov variable - i.e., a dynamical variable whose value varies monotonically as time increases. Incompatibility between certain assumed properties of a Lyapounov variable and semiboundedness of the spectrum of the Hamiltonian generating the quantum dynamics led MPC to formulate their theory in Liouville space. In the present paper it is proved, in a constructive way, that a Lyapounov variable can be found within the standard Hilbert space formulation of quantum mechanics and, hence, the MPC assumptions are more restrictive than necessary for the construction of such a quantity. Moreover, as in the MPC theory, the existence of a Lyapounov variable implies the existence of a transformation (the so called Λ-transformation) mapping the original quantum mechanical problem to an equivalent irreversible representation. In addition, it is proved that in the irreversible representation there exists a natural time observable splitting the Hilbert space at each $t > 0$ into past and future subspaces.

1 introduction

During the late 1970's and in the following decades a comprehensive theory of classical and quantum microscopic irreversibility has been developed by B. Misra, I. Prigogine and M. Courbage and various other contributors (see for exmple [10, 12, 13, 17, 2, 5, 1] and references therein). A central notion in this theory of irreversibility is that of a non-equilibrium entropy associated with the existence of Lyapounov variables for the dynamical system under consideration. In the case of a classical dynamical system one works with Koopman's formulation of classical mechanics in Hilbert space [8]. Associated with the dynamical system there exists a measure space $(\Omega, \mathcal{F}, \mu)$ such that Ω consists of all points belonging to a constant energy surface in phase space, $\mathcal{F}$ is a σ-algebra of measurable sets with respect to the measure μ which is taken to be the Liouville measure invariant under the Hamiltonian evolution. The Hamiltonian dynamics is given in terms of a one parameter dynamical group T_t mapping Ω onto itself with the condition that, for all t, T_t is measure preserving and injective. The

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Koopman Hilbert space is then the space $\mathcal{H} = L^2(\Omega, d\mu)$ of functions on Ω square integrable with respect to μ. The dynamics of the system is represented in $\mathcal{H}$ by a one-parameter unitary group $\{U_t\}_{t\in\mathbb{R}}$ induced by the group T_t via

$$(U_t\psi)(\omega) = \psi(T_{-t}\,\omega), \qquad \omega \in \Omega,\ \psi \in \mathcal{H}\,.$$

The generator of $\{U_t\}_{t\in\mathbb{R}}$ is the Liouvillian L

$$U_t = e^{-iLt}, \qquad t \in \mathbb{R}\,.$$

The generator L is, in general, an unbounded self-adjoint operator. For a Hamiltonian system it is given by

$$L\psi = i[H, \psi]_{pb}\,, \tag{1}$$

where the subscript *pb* stands for Poisson brackets and where Eq. (1) holds for all ψ for which its right hand side is well defined in $\mathcal{H}$.

A bounded, non-negative, self-adjoint operator M in $L^2(\Omega, d\mu)$ is called a *Lyapounov variable* essentially if it satisfies the condition that, for every $\psi \in \mathcal{H}$ the quantity

$$(\psi_t, M\psi_t) = (U_t\psi, MU_t\psi) \tag{2}$$

is a monotonically decreasing function of t. This monotonicity property of M allows, within the framework of the theory of irreversibity mentioned above, to define the notion of non-equilibrium entropy and the second law of thermodynamics as a fundamental dynamical principle. Of course, the monotonicity condition is not sufficient for the definition of non-equilibirium entropy and further conditions are introduced. These conditions will be discussed below.

In reference [10] a Lyapounov variable for a classical system is defined as a bounded operator M in $L^2(\Omega, d\mu)$ satisfying the conditions

1. M is a non-negative operator.
2. $\mathcal{D}(L)$, the domain of L, is stable under the action of M, i.e., $M\mathcal{D}(L) \subseteq \mathcal{D}(L)$.
3. $i[L, M] \subseteq -D$ where D is a non-negative, self-adjoint operator in $\mathcal{H}$.
4. $(\psi, D\psi) = 0$ iff $\psi(\omega) = const.$, $\omega \in \Omega$, a.e on Ω.

It is remarked in reference [10] that if, for a bounded operator M on $L^2(\Omega, d\mu)$, the quantity $(\psi_t, M\psi_t)$ has the required monotonicity property then M may be considered as a Lyapounov variable except for the fact that condition (2) above on the stability of $\mathcal{D}(L)$ may not be satisfied. In this respect an important observation for our purposes is that instability of $\mathcal{D}(L)$ under the action of M has direct consequences on the domain of definition of the commutator $i[L, M]$ appearing in condition (3).

In Koopman's Hilbert space formulation of classical mechanics all physical observables of the classical system have a natural represention as mutiliplicative operators in $L^2(\Omega, d\mu)$. By a theorem of Poincaré [18] there is no function on phase space that has a definite sign and is monotonically increasing under the Hamiltonian evolution. This leads to the conclusion that non-equilibrium entropy, or a Lyapounov variable, cannot be represented as a mutliplicative operator in the corresponding Hilbert space formulation of classical mechanics [10]. In fact, a

Lyapounov variable M does not commute with at least some of the operators of multiplication by phase space functions.

Consider now the framework of quantum mechanics where a physical system is described by a Hilbert space $\mathcal{H}$ and the quantum mechanical evolution is generated by a self-adjoint Hamiltonian operator H. Let $\mathcal{B}(\mathcal{H})$ be the space of bounded operators defined on $\mathcal{H}$ and let $M \in \mathcal{B}(\mathcal{H})$ be an operator in $\mathcal{H}$ representing a Lyapounov variable (corresponding to non-equilibrium entropy) and assume that

i) H is bounded from below; with no restriction of generality we may assume that $H \geq 0$,

ii) M is self-adjoint,

iii) $\mathcal{D}(H)$, the domain of H, is stable under the action of M,

iv) $i[H, M] \subseteq -D$ where D is self-adjoint on $\mathcal{H}$ and $D \geq 0$,

v) $[M, D] = 0$

Remarks: Condition (v) is to be interpreted as meaning that DM extends MD, i.e., $MD \subset DM$. In addition condition (iii) implies that the commutator $i[H, M]$ in condition (iv) is defined on $\mathcal{D}(H)$. Condition (iv) then implies that $\mathcal{D}(D) \supseteq \mathcal{D}(H)$.

Under a set of assumptions equivalent to conditions (i)-(v) above it has been proven by Misra, Prigogine and Courbage [12] that ptions (i)-(v) that $D \equiv 0$ and hence M cannot be a Lyapounov variable. The crucial element of the proof is the fact that H is bounded from below. The solution found by the authors of reference [12] is to work with the Liouvillian formulation of quantum mechanics where the quantum evolution is acting on the space of density operators and the generator of evolution is the Liouvillian L defined by

$$L\rho = [H, \rho]$$

with ρ a density operator. For example, if the Hamiltonian H satisfies the condition that $\sigma(H) = \sigma_{ac}(H) = \mathbb{R}^+$ then the Liouvillian L has an absolutely continuous spectrum of uniform (infinite) multiplicity consisting of all of $\mathbb{R}$. It is then possible to avoid the conclusions of the Poincare'-Misra no-go theorem and define M as a superoperator on the space of density operators satisfying in this space the conditions

$$i[L, M] \subseteq -D \leq 0, \qquad [M, D] = 0\,.$$

As mentioned above the monotnicity condition in the form of the existence of a Lyapounov variable M is not enough to identify M as an operator (in the classical case) or a superoperator (in the quantum case) representing non-equilibrium entropy. If M is a Lyapounov variable corresponding to non-equilibrium entropy one would also like to be able to use it in order to describe the process of decay of deviations from equilibrium for the physical system under consideration and recover the unidirectional nature of the evolution of such a system. A theory of transformation, via non-unitary mappings, between conservative dynamics represented by unitary evolution $\{U_t\}_{t\in\mathbb{R}}$ and dissipative dynamics represented by semigroup evolution $\{W_t\}_{t\in\mathbb{R}^+}$ has been developed by Misra, Prigogine and Courbage [13, 3, 6, 11, 17, 5] for systems with internal time operator T satisfying

$$U_{-t} T U_t = T + tI\,. \tag{3}$$

In this formalism the time operator T is canonically conjugate to the generator L of the unitary evolution group of the conservative dynamics, i.e. $U_t = \exp(-iLt)$ and

$$[L, T] = i\,. \tag{4}$$

For a system possessing internal time operator T it is possible to construct a Lyapounov variable as a positive monotonically decreasing operator function $M = M(T)$. One is then able to define a non-unitary transformation

$$\Lambda = \Lambda(T) = (M(T))^{1/2} \tag{5}$$

such that

$$\Lambda U_t = W_t \Lambda, \qquad t \geq 0 \tag{6}$$

where, as in the discussion above, W_t is a dissipative semigroup with

$$\|W_{t_2}\psi\| \leq \|W_{t_1}\psi\|, \qquad t_2 \geq t_1, \quad \psi \in \mathcal{H}$$

and

$$s - \lim_{t\to\infty} W_t = 0\,.$$

Note that Eq. (4) implies that $\sigma(L) = \mathbb{R}$ and $\sigma(T) = \mathbb{R}$ so that, in order for the Misra, Prigogine and Courbage formalism to work, it is required that the generator of evolution is unbounded from below.

The goal of the present paper is to show that it is possible to define the main objects and obtain many of the results of the Misra, Prigogine and Courbage theory within the standard formulation of quantum theory without ever invoking the need to work in a more generalized space such as Liouville space. It will be shown in Theorem 1 below that, under the same assumptions on the spectrum of the Hamiltonian as in the Misra, Prigogine and Courbage theory, the semiboundedness of the Hamiltonian does not hinder the possiblity of defining a Lyapounov variable for the Schrödinger evolution. Of course, in light of the no-go theorem discussed above, at least one of the conditions (i)-(v) above is not satisfied in the construction of this Lyapounov variable and, in fact, conditions (iii),(iv) and (v) do not hold in this construction. Detailed discussion of this point will be given elsewhere.

Theorem 1 concerning the existence of a Lyapounov variable M_F for forward (positive times) Schrödinger evolution is stated at the beginning of Section 2 and proved in Section 3.

Once the existence of the Lyapounov variable M_F is established one can proceed as in the Misra, Prigogine and Courbage theory and define a non-unitary Λ-transformation $\Lambda_F = M_F^{1/2}$ as in Eq. (5). It is to be emphasized, however, that the existence of a time operator satisfying Eq. (4) is not required in the construction of M_F and Λ_F and, in fact, since the spectrum of H is bounded from below, such a time operator does not exist.

It is shown in Section 2 that via the Λ-transformation Λ_F it is possible to establish a relation of the form given in Eq. (6), i.e., there exists a dissipative one-parameter continuous semigroup $\{Z(t)\}_{t\in\mathbb{R}^+}$ such that for $t \geq 0$ we have

$$\Lambda_F U(t) = Z(t)\Lambda_F, \quad t \geq 0\,,$$

one is then able to obtain the *irreversible representation* of the dynamics. This is done in Section 2. In the irreversible representation the dynamics of the system is unidirectional in time and is given in terms of the semigroup $\{Z(t)\}_{t\in\mathbb{R}^+}$.

It is an interesting fact that in the irreversible representation of the dynamics it is possible to find a positive semibounded operator T in $\mathcal{H}$ that can be intepreted as a natural time observable for the evolution of the system. The exact nature of this time observable and the main theorem concerned with its existence is discussed in Section 2. Of course, this operator is not a time operator in the sense of Eq. (3).

Following a statement in Section 2 of the main theorems proved in this paper and the discussion of their content, the proofs of these theorems are provided in Section 3. A short summary is provided in Section 4.

2 Main theorems and results

The three main theorems in this section, and the discussion accompanying them, provide the main results of the present paper. We start with the existence of Lyapounov variables for Schrödinger evolution.

Theorem 1 *Assume that:*

a) *$\mathcal{H}$ is a separable Hilbert space and $\{U(t)\}_{t\in\mathbb{R}}$ is a unitary evolution group defined on $\mathcal{H}$,*

b) *the generator H of $\{U(t)\}_{t\in\mathbb{R}}$ is self-adjoint on a dense domain $\mathcal{D}(H)\subset\mathcal{H}$ and $\sigma(H)=\sigma_{ac}(H)=\mathbb{R}^+$,*

c) *The spectrum $\sigma(H)$ is of multiplicity one (see remark below).*

Let $\{\phi_E\}_{E\in\mathbb{R}^+}$ be a complete set of improper eigenvectors of H corrsponding to the spectrum of H. We shall use the Dirac notation and denote $\{|E\rangle\}_{E\in\mathbb{R}^+}\equiv\{\phi_E\}_{E\in\mathbb{R}^+}$. Then, under the assumptions (a)-(c) above there exists a self-adjoint, contractive, injective, non-negative operator $M_F:\mathcal{H}\mapsto\mathcal{H}$

$$M_F := \frac{-1}{2\pi i}\int_0^\infty dE'\int_0^\infty dE\,|E'\rangle\,\frac{1}{E'-E+i0^+}\,\langle E| \tag{7}$$

such that $\mathrm{Ran}\,M_F\subset\mathcal{H}$ is dense in $\mathcal{H}$ and M_F is a Lyapounov variable for the Schrödinger evolution in the forward direction, i.e., for every $\psi\in\mathcal{H}$ we have

$$(\psi_{t_2}, M_F\,\psi_{t_2})\le(\psi_{t_1}, M_F\,\psi_{t_1}),\qquad t_2>t_1\ge 0,\quad \psi_t=U(t)\psi=e^{-iHt}\psi,\ t\ge 0 \tag{8}$$

and

$$\lim_{t\to\infty}(\psi_t, M_F\,\psi_t)=0\,. \tag{9}$$

□

Remark: Assumption (c) above is made for simplicity of proof and exposition. The result has immediate generalization to a spectrum of any finite multiplicity. The case of infinite multiplicity will be cosidered separately elsewhere.

Following the proof of the existence of the Lyapounov variable M_F we can proceed as in the Misra, Prigogine and Courbage theory and obtain a non-unitary Λ transformation via the definition $\Lambda_F := M_F^{1/2}$. We then have the following theorem

Theorem 2 *Let $\Lambda_F := M_F^{1/2}$. Then $\Lambda_F : \mathcal{H} \mapsto \mathcal{H}$ is positive, contractive and quasi-affine map, i.e., it is a positive, contractive, injective operator such that $Ran\,\Lambda_F$ is dense in $\mathcal{H}$. Furthermore, there exists a continuous, strongly contractive, one parameter semigroup $\{Z(t)\}_{t\in\mathbb{R}^+}$ such that*

$$\|Z(t_2)\psi\| \leq \|Z(t_1)\psi\|, \quad t_2 \geq t_1 \geq 0, \qquad s-\lim_{t\to\infty} Z(t) = 0\,. \tag{10}$$

and the following intertwining relation holds

$$\Lambda_F U(t) = Z(t)\Lambda_F, \qquad U(t) = e^{-iHt}, \quad t \geq 0\,. \tag{11}$$

□

Taking the adjoint of Eq. (11) we obtain the intertwining relation

$$U(-t)\Lambda_F = \Lambda_F Z^*(t), \quad t \geq 0\,. \tag{12}$$

Let $\mathcal{L}(\mathcal{H})$ be the set of linear operators in $\mathcal{H}$. For $X \in \mathcal{L}(\mathcal{H})$ denote $X_{\Lambda_F} := \Lambda_F X \Lambda_F$ and consider the set of all self-adjoint operators $X \in \mathcal{L}(\mathcal{H})$ such that $\mathcal{D}(X_{\Lambda_F})$ is dense in $\mathcal{H}$ i.e., such that $\Lambda_F^{-1}\mathcal{D}(X)$ is dense in $\mathcal{H}$. Using Eqns. (11) and (12) we obtain

$$U(-t)X_{\Lambda_F}U(t) = U(-t)\Lambda_F X \Lambda_F U(t) = \Lambda_F Z^*(t) X Z(t)\Lambda_F, \quad t \geq 0\,. \tag{13}$$

For $\varphi, \psi \in \mathcal{H}$ denote $\varphi_{\Lambda_F} = \Lambda_F\varphi$ and $\psi_{\Lambda_F} = \Lambda_F\psi$. Then using Eq. (13) implies that

$$(\varphi, U(-t)X_{\Lambda_F}U(t)\psi) = (\varphi, \Lambda_F Z^*(t)XZ(t)\Lambda_F\psi) = (\varphi_{\Lambda_F}, Z^*(t)XZ(t)\psi_{\Lambda_F}), \quad t \geq 0\,. \tag{14}$$

We shall assume that *each and every relevant physical observable of the original problem has a representation in the form $X_{\Lambda_F} = \Lambda_F X \Lambda_F$ for some self-adjoint $X \in \mathcal{L}(\mathcal{H})$*. Then, since the left hand side of Eq. (14) corresponds to the original quantum mechanical problem, the right hand side of this equation constitutes a new representation of the original problem in terms of the correspondence

$$\begin{aligned} \psi \quad &\longrightarrow \quad \psi_{\Lambda_F} = \Lambda_F\psi \\ U(t) \quad &\longrightarrow \quad Z(t) = \Lambda_F\, U(t)\Lambda_F^{-1}, \quad t \geq 0 \\ X_{\Lambda_F} \quad &\longrightarrow \quad X = \Lambda_F^{-1} X_{\Lambda_F} \Lambda_F^{-1}\,. \end{aligned}$$

Considering the fact that on the right hand side of Eq. (14) the dynamics is given in terms of the semigroup $\{Z(t)\}_{t\in\mathbb{R}^+}$ we may call the right hand side of Eq. (14) the *irreversible representation* of the problem. The left hand side of that equation is then the *reversible representation* (or the standard representation).

It is an interesting fact that in the irreversible representation of a quantum mechanical problem, as in the right hand side of Eq. (14), one can find a self-adjoint operator T with continuous spectrum $\sigma(T) = ([0, \infty))$ such that for every $t \geq 0$ the spectral projections on the spectrum of T naturally divide the Hilbert space $\mathcal{H}$ into a direct sum of a *past subspace at time t* and a *future subspace at time t*. Specifically, we have the following theorem:

Theorem 3 *Let $\mathcal{B}(\mathbb{R}^+)$ be the Borel σ-algebra generated by open subsets of $\mathbb{R}^+$ and $\mathcal{P}(\mathcal{H})$ be the set of orthogonal projections in $\mathcal{H}$. There exists a semi-bounded, self-adjoint operator $T : \mathcal{D}(T) \mapsto \mathcal{H}$ defined on a dense domain $\mathcal{D}(T) \subset \mathcal{H}$ with continuous spectrum $\sigma(T) = [0, \infty)$ and corresponding spectral measure $\mu_T : \mathcal{B}(\mathbb{R}^+) \mapsto \mathcal{P}(\mathcal{H})$ such that for each $t \geq 0$*

$$\mu_T([0, t])\mathcal{H} = [Z(t), Z^*(t)]\mathcal{H} = Ker\, Z(t), \qquad t \geq 0$$

and

$$\mu_T([t,\infty))\mathcal{H} = Z^*(t)Z(t)\mathcal{H} = (Ker\, Z(t))^\perp, \qquad t \geq 0\,.$$

In particular, for $0 < t_1 < t_2$ *we have* $Ker\, Z(t_1) \subset Ker\, Z(t_2)$. *For* $t = 0$ *we have* $Ker\, Z(0) = \{0\}$ *and finally* $\lim_{t\to\infty} Ker\, Z(t) = \mathcal{H}$. □

Denote the orthogonal projection on $Ker\, Z(t)$ by $P_{t]}$ and the orthogonal projection on $(Ker\, Z(t))^\perp$ by $P_{[t}$. From Theorem 3 we have for $t \geq 0$

$$P_{t]} = [Z(t), Z^*(t)], \qquad P_{[t} = Z^*(t)Z(t), \quad t \geq 0\,.$$

The projection $P_{t]}$ will be called below the *projection on the past subspace at time* t. The projection $P_{[t}$ will be called the *projection on the future subspace at time* t. In accordance we will call $\mathcal{H}_{t]} := Ran\, P_{t]} = Ker\, Z(t)$ the *past subspace at time* t and $\mathcal{H}_{[t} := Ran\, P_{[t} = (Ker\, Z(t))^\perp$ the *future subspace at time* t. The origin of the terminology used here can be found in Eq. (14). Using the notation for the projection on $Ker\, Z(t)$ we observe that this equation may be written in the form

$$(\varphi, U(-t)X_{\Lambda_F}U(t)\psi) = (P_{[t}\, \varphi_{\Lambda_F}, Z^*(t)XZ(t)P_{[t}\, \psi_{\Lambda_F}), \quad t \geq 0\,,$$

and denoting $\varphi^+_{\Lambda_F}(t) := P_{[t}\, \varphi_{\Lambda_F} = P_{[t}\Lambda_F\varphi$ and $\psi^+_{\Lambda_F}(t) := P_{[t}\, \psi_{\Lambda_F} = P_{[t}\Lambda_F\psi$ we can write in short

$$(\varphi, U(-t)X_{\Lambda_F}U(t)\psi) = (\varphi^+_{\Lambda_F}(t), Z^*(t)XZ(t)\psi^+_{\Lambda_F}(t)), \quad t \geq 0\,. \tag{15}$$

Note that in the irreversible representation on the right hand side of Eq. (15) only the projection of φ_{Λ_F} and ψ_{Λ_F} on the future subspace $\mathcal{H}_{[t}$ at time t is relevant for the calculation of all matrix elements and expectation values for times $t' \geq t \geq 0$. In other words, at time t the subspace $\mathcal{H}_{t]} = P_{t]}\mathcal{H}$ already belongs to the past and is irrelevant for calculations related to the future evolution of the system. We see that in the irreversible representation the spectral projections of the operator T provide the time ordering of the evolution of the system. Following these observations it is natural to call T a *time observable* for the irreversible representation. Note, in particular, that since $M_F = \Lambda_F^2$ we have $\Lambda_F^{-1}M_F\Lambda_F^{-1} = I$ and if we plug this relation in Eq. (14) or Eq. (15) and take $\varphi = \psi$ we obtain

$$\begin{aligned}(\psi_t, M_F\, \psi_t) = (\psi, U(-t)M_FU(t)\psi) = (\psi_{\Lambda_F}, Z^*(t)Z(t)\psi_{\Lambda_F}) = \\ = (\psi_{\Lambda_F}, P_{[t}\, \psi_{\Lambda_F}) = (\psi_{\Lambda_F}, \mu_T([t,\infty))\psi_{\Lambda_F}), \quad t \geq 0\,,\end{aligned}$$

thus we have direct correspondence between the Lyapounov variable M_F in the reversible representation of the problem and the time observable in the irreversible representation.

3 Proofs of Main results

The basic mechanism underlying the proofs of Theorem 1 and Theorem 2 is a fundamental intertwining relation, via a quasi-affine mapping, between the unitary Schrödinger evolution in physical space $\mathcal{H}$ and semigroup evolution in Hardy space of the upper half-plane $\mathcal{H}^2(\mathbb{C}^+)$ or the isomorphic space $\mathcal{H}^2_+(\mathbb{R})$ of boundary values on $\mathbb{R}$ of functions in $\mathcal{H}^2_+(\mathbb{C})$. Hence we begin our proof with a few facts concerning Hardy space functions which are used below.

Denote by $\mathbb{C}^+$ the upper half of the complex plane. The Hardy space $\mathcal{H}^2(\mathbb{C}^+)$ of the upper half-plane consists of functions analytic in $\mathbb{C}^+$ and satisfying the condition that for any $f \in \mathcal{H}^2(\mathbb{C}^+)$ there exists a constant $C_f > 0$ such that

$$\sup_{y>0} \int_{-\infty}^{\infty} dx \, |f(x+iy)|^2 < C_f \, .$$

In a similar manner the Hardy space $\mathcal{H}^2(\mathbb{C}^-)$ consists of functions analytic in the lower half-plane $\mathbb{C}^-$ and satisfying the condition that for any $g \in \mathcal{H}^2(\mathbb{C}^-)$ there exists a constant $C_g > 0$ such that

$$\sup_{y>0} \int_{-\infty}^{\infty} dx \, |f(x-iy)|^2 < C_g \, .$$

Hardy space functions have non-tangential boundary values a.e. on $\mathbb{R}$. In particular, for $f \in \mathcal{H}^2(\mathbb{C}^+)$ there exists a function $\tilde{f} \in L^2(\mathbb{R})$ such that a.e on $\mathbb{R}$ we have

$$\lim_{y \to 0^+} f(x+iy) = \tilde{f}(x), \quad x \in \mathbb{R} \, .$$

a similar limit from below the real axis holds for functions in $\mathcal{H}^2(\mathbb{C}^-)$. In fact $\mathcal{H}^2(\mathbb{C}^\pm)$ are Hilbert spaces with scalar product given by

$$(f,g)_{\mathcal{H}^2(\mathbb{C}^\pm)} = \lim_{y \to 0^+} \int_{-\infty}^{\infty} dx \, \overline{f(x \pm iy)} g(x \pm iy) = \int_{-\infty}^{\infty} dx \, \overline{\tilde{f}(x)} \tilde{g}(x), \quad f,g \in \mathcal{H}^2(\mathbb{C}^\pm) \, ,$$

where $\tilde{f}$, $\tilde{g}$ are the boundary value functions of f and g respectively. The spaces of boundry values on $\mathbb{R}$ of functions in $\mathcal{H}^2(\mathbb{C}^\pm)$ are then Hilbert spaces isomorphic to $\mathcal{H}^2(\mathbb{C}^\pm)$ which we denote by $\mathcal{H}^2_\pm(\mathbb{R})$.

A Theorem of Titchmarsh [26] states that Hardy space functions can be reconstructed from their boundary value functions. If $\tilde{f}_\pm \in \mathcal{H}^2_\pm(\mathbb{R})$ is a boundary value function of a function $f \in \mathcal{H}^2(\mathbb{C}^\pm)$ then one has

$$f(z) = \mp \frac{1}{2\pi i} \int_{-\infty}^{\infty} dx \, \frac{\tilde{f}(x)}{z-x} \tag{16}$$

where the minus sign corresponds to functions in $\mathcal{H}^2(\mathbb{C}^+)$ and the plus sign corresponds to functions in $\mathcal{H}^2(\mathbb{C}^-)$. In addition we shall make use below of the fact that

$$\mathcal{H}^2_+(\mathbb{R}) \oplus \mathcal{H}^2_-(\mathbb{R}) = L^2(\mathbb{R}) \, .$$

It can be shown that for functions in $\mathcal{H}^2(\mathbb{C}^\pm)$ have radial limits of order $o(z^{-1/2})$ as $|z|$ goes to infinity in the upper and lower half-plane repectively. As a consequence, if we denote by P_+ and P_- the projections of $L^2(\mathbb{R})$ on $\mathcal{H}^2_+(\mathbb{R})$ and $\mathcal{H}^2_-(\mathbb{R})$ respectively, Eq. (16) and the existence of boundary value functions in $\mathcal{H}^2_\pm(\mathbb{R})$ provides us with explicit expressions for these projections in the form

$$(P_\pm f)(\sigma') = \mp \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\sigma \, \frac{1}{\sigma' - \sigma + i0^+} f(\sigma), \qquad f \in L^2(\mathbb{R}), \ \ \sigma' \in \mathbb{R} \, . \tag{17}$$

The literature on Hardy spaces is quite rich. Additional important properties of Hardy spaces can be found in [9, 4, 7]. For the vector valued case see, for example, [21].

Define a family $\{u(t)\}_{t\in\mathbb{R}}$ of unitary multiplicative operators $u(t): L^2(\mathbb{R}) \mapsto L^2(\mathbb{R})$ by

$$[u(t)f](\sigma) = e^{-i\sigma t} f(\sigma), \qquad f \in L^2(\mathbb{R}), \ \ \sigma \in \mathbb{R}\,.$$

The family $\{u(t)\}_{t\in\mathbb{R}}$ forms a one parameter group of multiplicative operators in $L^2(\mathbb{R})$. Let P_+ be the orthogonal projection of $L^2(\mathbb{R})$ on $\mathcal{H}^2_+(\mathbb{R})$. A *Toeplitz operator* with symbol $u(t)$ [21, 14, 15] is an operator $T_u(t): \mathcal{H}^2_+(\mathbb{R}) \mapsto \mathcal{H}^2_+(\mathbb{R})$ defined by

$$T_u(t) f = P_+ u(t) f, \qquad f \in \mathcal{H}^2_+(\mathbb{R})\,.$$

The set $\{T_u(t)\}_{t\in\mathbb{R}^+}$ forms a strongly continuous, contractive, one parameter semigroup on $\mathcal{H}^2_+(\mathbb{R})$ satisfying

$$\|T_u(t_2) f\| \leq \|T_u(t_1) f\|, \qquad t_2 \geq t_1 \geq 0, \ \ f \in \mathcal{H}^2_+(\mathbb{R})\,, \tag{18}$$

and

$$s - \lim_{t\to\infty} T_u(t) = 0\,. \tag{19}$$

Below we shall make frequent use of quasi-affine mappings. The definition of this class of maps is as follows:

Definition 1 (quasi-affine map) *A quasi-affine map from a Hilbert space $\mathcal{H}_1$ into a Hilbert space $\mathcal{H}_0$ is a linear, injective, continuous mapping of $\mathcal{H}_1$ into a dense linear manifold in $\mathcal{H}_0$. If $A \in \mathcal{B}(\mathcal{H}_1)$ and $B \in \mathcal{B}(\mathcal{H}_0)$ then A is a quasi-affine transform of B if there is a quasi-affine map $\theta : \mathcal{H}_1 \mapsto \mathcal{H}_0$ such that $\theta A = B\theta$.* □

Concerning quasi-affine maps we have the following two important facts (see, for example [16]):

I) If $\theta : \mathcal{H}_1 \mapsto \mathcal{H}_0$ is a quasi-affine mapping then $\theta^* : \mathcal{H}_0 \mapsto \mathcal{H}_1$ is also quasi-affine, that is, θ^* is one to one, continuous and its range is dense in $\mathcal{H}_1$.

II) If $\theta_1 : \mathcal{H}_0 \mapsto \mathcal{H}_1$ is quasi-affine and $\theta_2 : \mathcal{H}_1 \mapsto \mathcal{H}_2$ is quasi-affine then $\theta_2\theta_1 : \mathcal{H}_0 \mapsto \mathcal{H}_2$ is quasi-affine.

We can now turn to the proof of Theorem 1:

Proof of Theorem 1:

Assume that (a)-(c) in the statement of Theorem 1 hold. A slight variation of a theorem first proved in [22], and subsequently used in the study of resonances in [22, 23, 25] and time observables in quantum mechanics in [24], states that there exists a mapping $\Omega_f : \mathcal{H} \mapsto \mathcal{H}^2_+(\mathbb{R})$ such that

α) Ω_f is a contractive quasi-affine mapping of $\mathcal{H}$ into $\mathcal{H}^2_+(\mathbb{R})$.

β) For $t \geq 0$, the Schrödinger evolution $U(t)$ is a quasi-affine transform of the Toeplitz operator $T_u(t)$. For every $t \geq 0$ and $g \in \mathcal{H}$ we have

$$\Omega_f U(t) g = T_u(t) \Omega_f g, \qquad t \geq 0, \ \ g \in \mathcal{H}\,. \tag{20}$$

(here the subscript f in Ω_f designates forward time evolution). By (I) above the adjoint $\Omega_f^*: \mathcal{H}_+^2(\mathbb{R}) \mapsto \mathcal{H}$ is a quasi-affine map. Hence, Ω_f^* is continuous and one to one and $Ran\,\Omega_f^*$ is dense in $\mathcal{H}$. Define the operator $M_F: \mathcal{H} \mapsto \mathcal{H}$ by

$$M_F := \Omega_f^* \Omega_f\,.$$

By (II) above and the fact that Ω_f, Ω_f^* are quasi-affine we get that M_F is a quasi-affine mapping from $\mathcal{H}$ into $\mathcal{H}$. Therefore M_F is continuous and injective and $Ran\,M_F$ is dense in $\mathcal{H}$. Obviously M_F is symmetric and, since Ω_f and Ω_f^* are bounded, then $Dom\,M_F = \mathcal{H}$ and we conclude that M_F is self-adjoint. Since Ω_f and Ω_f^* are both contractive then M_F is contractive. In fact, it is shown in [24] that $\|M_F\| = 1$.

Remark: It is to be noted that the operator M_F already appears in reference [24] in a slightly different context. Indeed, M_F is identical to the inverse T_F^{-1} of the operator T_F called the *time observable* in that paper.

Taking the adjoint of Eq. (20) we obtain

$$U(-t)\Omega_f^* g = \Omega_f^*(T_u(t))^* g, \qquad t \geq 0,\quad g \in \mathcal{H}_+^2(\mathbb{R}), \qquad t \geq 0,\quad g \in \mathcal{H}_+^2(\mathbb{R})\,, \tag{21}$$

we obtain from Eqns. (20) and (21) an expression for the Heisenberg evolution of M_F

$$U(-t)M_F U(t) = U(-t)\Omega_f^*\Omega_f U(t) = \Omega_f^*(T_u(t))^* T_u(t)\Omega_f\,.$$

For any $\psi \in \mathcal{H}$ we then get

$$(\psi, U(-t)M_F U(t)\psi) = (\psi, \Omega_f^*(T_u(t))^* T_u(t)\Omega_f\psi) = \|T_u(t)\Omega_f\psi\|^2, \qquad t \geq 0,\quad \psi \in \mathcal{H}\,.$$

The fact that M_F is a Lyapounov variable, i.e., the validity of Eqns. (8) and (9) then follows immediately from Eqns. (18) and (19).

We are left with the task of showing that M_F can be expressed in the form given by Eq. (7). For this we need a more explicit expression for the map Ω_f. It follows from assumptions (a)-(c) in Theorem 1 that there exists a unitary mapping $U: \mathcal{H} \mapsto L^2(\mathbb{R}^+)$ of $\mathcal{H}$ into its spectral representation on the spectrum of H (energy representation for H). The energy representation is obtained by finding a complete set of improper eigenvectors $\{\phi_E\}_{E\in\mathbb{R}^+}$ of H, corresponding to the (by assumption absolutely continuous) spectrum of H. Using the Dirac notation $\{\phi_E\}_{E\in\mathbb{R}^+} \equiv \{|E\rangle\}_{E\in\mathbb{R}^+}$ we have

$$(U\psi)(E) = \langle E|\psi\rangle = \psi(E), \qquad E \in \mathbb{R}^+,\quad \psi \in \mathcal{H}\,. \tag{22}$$

the inverse of U is given by

$$U^* f = \int_0^\infty dE\,|E\rangle\,\psi(E), \qquad \psi \in L^2(\mathbb{R}^+)\,. \tag{23}$$

Let $P_{\mathbb{R}^+}: L^2(\mathbb{R}) \mapsto L^2(\mathbb{R})$ be the orthogonal projection in $L^2(\mathbb{R})$ on the subspace of functions supported on $\mathbb{R}^+$ and define the inclusion map $I: L^2(\mathbb{R}^+) \mapsto L^2(\mathbb{R})$ by

$$(If)(\sigma) = \begin{cases} f(\sigma), & \sigma \geq 0 \\ 0, & \sigma < 0 \end{cases}, \qquad \sigma \in \mathbb{R}\,.$$

Then the inverse $I^{-1}: P_{\mathbb{R}^+}L^2(\mathbb{R}) \mapsto L^2(\mathbb{R}^+)$ is well defined on $P_{\mathbb{R}^+}L^2(\mathbb{R})$. Let $\theta : \mathcal{H}^2_+(\mathbb{R}) \mapsto L^2(\mathbb{R}^+)$ be given by

$$\theta f = I^{-1} P_{\mathbb{R}^+} f, \qquad f \in \mathcal{H}^2_+(\mathbb{R})\,.$$

By a theorem of Van-Winter [27] θ is a contractive quasi-affine mapping of $\mathcal{H}^2_+(\mathbb{R})$ into $L^2(\mathbb{R}^+)$. The adjoint map $\theta^* : L^2(\mathbb{R}^+) \mapsto \mathcal{H}^2_+(\mathbb{R})$ is then also a contractive quasi-affine map. An explicit expression for θ^* is given in [22, 23]

$$\theta^* f = P_+ I f, \qquad f \in L^2(\mathbb{R}^+)\,.$$

It is shown in [22, 23] that the maps Ω_f and Ω_f^* are given by

$$\Omega_f = \theta^* U, \qquad \Omega_f^* = U^* \theta\,.$$

From the definition of the embedding map I and the expression for P_+ in Eq. (17) we get

$$(\theta^* f)(\sigma) = \frac{-1}{2\pi i} \int_0^\infty dE\, \frac{1}{\sigma - E + i0^+} f(E), \qquad \sigma \in \mathbb{R},\ f \in L^2(\mathbb{R}^+)\,. \tag{24}$$

Combining Eqns. (22), (23) and Eq. (24) we finally obtain

$$M_F = \Omega_f^* \Omega_f = \frac{-1}{2\pi i} \int_0^\infty dE' \int_0^\infty dE\, |E'\rangle \frac{1}{E' - E + i0^+} \langle E|\,.$$

■

We now proceed to the proof of the second main result of this paper:

Proof of Theorem 2

Since M_F is a bounded positive operator its positive square root Λ_F is well defined and unique [20] and we set $\Lambda_F := M_F^{1/2} = (\Omega_f^* \Omega_f)^{1/2}$. Moreover, since

$$M_F \mathcal{H} = \Lambda_F \Lambda_F \mathcal{H} \subseteq \Lambda_F \mathcal{H}\,,$$

and since $Ran\, M_F$ is dense in $\mathcal{H}$ we conclude that $Ran\, \Lambda_F$ is dense in $\mathcal{H}$. Furthermore, since $M_F = \Lambda_F^2$ is one to one then Λ_F must also be one to one. We can summarize the findings above by stating that the fact that M_F is positive, one to one and quasi-affine implies the same properties for Λ_F. Since M_F is contractive and since for every $\psi \in \mathcal{H}$ we have $(\psi, M_F\, \psi) = \|\Lambda_F \psi\|^2$ we conclude that Λ_F is also contractive.

Define a mapping $\tilde{R} : \mathcal{D}(\tilde{R}) \mapsto \mathcal{H}^2_+(\mathbb{R})$ with $\mathcal{D}(\tilde{R}) \subseteq \mathcal{H}$ and

$$\tilde{R} := \Omega_f (\Omega_f^* \Omega_f)^{-1/2} = \Omega_f \Lambda_F^{-1}\,. \tag{25}$$

Obviously $\mathcal{D}(\tilde{R}) \supseteq Ran\, \Lambda_F \supset Ran\, M_F$ so that $\tilde{R}$ is defined on a dense set in $\mathcal{H}$. For any $f \in \mathcal{D}(\tilde{R})$ we have

$$\begin{aligned} \|\tilde{R} f\|^2 &= (\tilde{R} f, \tilde{R} f) = (\Omega_f (\Omega_f^* \Omega_f)^{-1/2} f, \Omega_f (\Omega_f^* \Omega_f)^{-1/2} f) = \\ &= ((\Omega_f^* \Omega_f)^{-1/2} f, \Omega_f^* \Omega_f (\Omega_f^* \Omega_f)^{-1/2} f) = ((\Omega_f^* \Omega_f)^{-1/2} f, (\Omega_f^* \Omega_f)^{1/2} f) = \|f\|^2\,, \end{aligned} \tag{26}$$

hence $\tilde{R}$ is isometric on a dense set in $\mathcal{H}$ and can be extended to an isometric map $R : \mathcal{H} \mapsto \mathcal{H}^2_+(\mathbb{R})$ such that

$$R^* R = I_{\mathcal{H}}\,.$$

From Eq. (26) we see that on the dense set $Ran\,\tilde{R} \subset \mathcal{H}^2_+(\mathbb{R})$ we have

$$\tilde{R}^* f = (\Omega_f^* \Omega_f)^{-1/2} \Omega_f^* f = \Lambda_F^{-1} \Omega_f^* f, \qquad f \in Ran\,\tilde{R}$$

and the adjoint R^* of R is an extension of $\tilde{R}^*$ to $\mathcal{H}^2_+(\mathbb{R})$. Note that the definition of $\tilde{R}$ implies that $Ran\,\tilde{R} \subseteq Ran\,\Omega_f$. Hence, for any $g \in Ran\,\Omega_f$ we have

$$\tilde{R}^* g = (\Omega_f^* \Omega_f)^{-1/2} \Omega_f^* g = (\Omega_f^* \Omega_f)^{-1/2} \Omega_f^* \Omega_f \Omega_f^{-1} g = (\Omega_f^* \Omega_f)^{1/2} \Omega_f^{-1} = \Lambda_f \Omega_f^{-1} g\,. \tag{27}$$

Thus on the dense set $Ran\,\Omega_f \subset \mathcal{H}^2_+(\mathbb{R})$ we have

$$R\,R^* g = [\Omega_f (\Omega_f^* \Omega_f)^{-1/2}][(\Omega_f^* \Omega_f)^{1/2} \Omega_f^{-1}] g = g$$

and by continuity we obtain

$$R\,R^* = I_{\mathcal{H}^2_+(\mathbb{R})}$$

and hence $R : \mathcal{H} \mapsto \mathcal{H}^2_+(\mathbb{R})$ is, in fact, a unitary map.

Now define

$$Z(t) := \Lambda_F U(t) \Lambda_F^{-1}, \qquad t \geq 0\,.$$

Obviously, $Z(t)$ is well defined on $Ran\,\Lambda_F$ for any $t \geq 0$. Moreover, using the definition of $\tilde{R}$ from Eq. (25) and Eqns. (27), (20) we get

$$\begin{aligned} RZ(t)R^* g = \Omega_f \Lambda_F^{-1} Z(t) \Lambda_F \Omega_f^{-1} g = [\Omega_f \Lambda_F^{-1}]\,[\Lambda_F U(t) \Lambda_F^{-1}]\,[\Lambda_F \Omega_f^{-1}] g = \\ = \Omega_f U(t) \Omega_f^{-1} g = T_u(t) g, \quad t \geq 0, \quad g \in Ran\,\Omega_f \subset \mathcal{H}^2_+(\mathbb{R})\,. \end{aligned}$$

Then on the dense subset $R^* \Lambda_F \mathcal{H} \subset \mathcal{H}$ we have $Z(t) = R^* T_u(t) R$ and since R and $T_u(t)$ are bounded we are able by continuity to extend the domain of definition of $Z(t)$ to all of $\mathcal{H}$ and obtain

$$RZ(t)R^* = T_u(t), \quad Z(t) = R^* T_u(t) R, \quad t \geq 0\,. \tag{28}$$

From the unitarity of R, the fact that $\{T_u(t)\}_{t \in \mathbb{R}^+}$ is a continuous, strongly contractive, one parameter semigroup and Eqns. (18), (19) we conclude that $\{Z(t)\}_{t \in \mathbb{R}^+}$ is a continuous, strongly contractive, one parameter semigroup and Eqns. (10) and (11) hold. ■

Proof of Theorem 3:

The main results of Theorem 3 are consequences of the following lemma:

Lemma 1 *For every $t \geq 0$ the operator $T_u(t) : \mathcal{H}^2_+(\mathbb{R}) \mapsto \mathcal{H}^2_+(\mathbb{R})$ is isometric and we have*

$$Ran\,(T_u(t))^* = (Ker\,T_u(t))^{\perp} \tag{29}$$

and

$$T_u(t)(T_u(t))^* = I_{\mathcal{H}^2_+(\mathbb{R})}, \quad t \geq 0\,.$$

Furthermore, if $\hat{P}_{t]} : \mathcal{H}^2_+(\mathbb{R}) \mapsto \mathcal{H}^2_+(\mathbb{R})$ *is the orthogonal projection on* $Ker\, T_u(t)$ *and* $\hat{P}_{[t}$ *is the orthogonal projection on* $(Ker\, T_u(t))^\perp$ *then*

$$\hat{P}_{t]} = [T_u(t), (T_u(t))^*], \quad t \geq 0$$

and

$$\hat{P}_{[t} = (T_u(t))^* T_u(t), \quad t \geq 0\,.$$

Moreover, we have

$$\hat{P}_{t_1]}\hat{P}_{t_2]} = \hat{P}_{t_1]}, \quad t_2 \geq t_1 \geq 0, \qquad Ran\, \hat{P}_{t_1]} \subset Ran\, \hat{P}_{t_2]}, \quad t_2 > t_1 \tag{30}$$

and

$$\hat{P}_{0]} = 0, \qquad \lim_{t\to\infty} \hat{P}_{t]} = I_{\mathcal{H}^2_+(\mathbb{R})}\,.$$

□

Proof of Lemma 1:

Recall that $T_u(t)f = P_+u(t)f$ for $t \geq 0$ and $f \in \mathcal{H}^2_+(\mathbb{R})$. Since $\mathcal{H}^2_+(\mathbb{R})$ is stable under $u^*(t) = u(-t)$ for $t \geq 0$, i.e., $u(-t)\mathcal{H}^2_+(\mathbb{R}) \subset \mathcal{H}^2_+(\mathbb{R})$ (as one can see, for example, by using the Paley-Wiener theorem [19]), we find that for any $f, g \in \mathcal{H}^2_+(\mathbb{R})$ we have

$$(g, T_u(t)f) = (g, P_+u(t)f) = (u(-t)g, f) = (P_+u(-t)g, f) = (T_{u^*}(t)g, f) = ((T_u(t))^*g, f)\,.$$

Therefore

$$(T_u(t))^*g = u(-t)g, \quad t \geq 0, \quad g \in \mathcal{H}^2_+(\mathbb{R})\,. \tag{31}$$

Since $u(-t)$ is unitary on $L^2(\mathbb{R})$ Eq. (31) implies that $(T_u(t))^*$ is isometric on $\mathcal{H}^2_+(\mathbb{R})$. The same equation implies also that

$$(T_u(t)(T_u(t))^*f = P_+u(-t)u(t)f = P_+f = f, \quad t \geq 0, \quad f \in \mathcal{H}^2_+(\mathbb{R})\,. \tag{32}$$

Consider now the operator $A(t) := (T_u(t))^*T_u(t)$ for $t \geq 0$. Since $Dom\, T_u(t) = \mathcal{H}^2_+(\mathbb{R})$ we have that $A(t)$ is self-adjoint. In addition Eq. (32 implies that

$$(A(t))^2 = [(T_u(t))^*T_u(t)][(T_u(t))^*T_u(t)] = (T_u(t))^*T_u(t) = A(t), \quad t \geq 0\,,$$

so that $A(t)$ is an orthogonal projection in $\mathcal{H}^2_+(\mathbb{R})$. Of course, for any $u \in Ker\, T_u(t)$ we have $A(t)u = 0$, hence $Ran\, A(t) \subseteq Ker\, T_u(t)$. Assume that there is some $v \in (Ran\, A(t))^\perp \cap (Ker\, T_u(t))^\perp$ with $v \neq 0$. Then we must have $A(t)v = 0$, but since $T_u(t)v \neq 0$ and since $(T_u(t))^*$ is an isometry we obtain a contradiction. Therefore $Ran\, A(t) = (Ker\, T_u(t))^\perp$ and $\hat{P}_{[t} = A(t) = (T_u(t))^*T_u(t)$. Taking into account Eq. (32) we obtain also $\hat{P}_{t]} = I - \hat{P}_{[t} = [T_u(t), (T_u(t))^*]$.

To prove Eq. (29) we note that since $(T_u(t))^*$ is isometric its range is a close subspace of $\mathcal{H}^2_+(\mathbb{R})$ and, moreover, $(Ran\,(T_u(t))^*)^\perp \supseteq Ker\, T_u(t)$. This is a result of the fact that if $u \in Ker\, T_u(t)$ then $(u, (T_u(t))^*v) = (T_u(t)u, v) = 0$, $\forall v \in \mathcal{H}^2_+(\mathbb{R})$. On the other hand, if u is orthogonal to $Ran\,(T_u(t))^*$ i.e., u is such that $(u, (T_u(t))^*v) = 0$, $\forall v \in \mathcal{H}^2_+(\mathbb{R})$ then $(T_u(t)u, v) = 0$, $\forall v \in \mathcal{H}^2_+(\mathbb{R})$ so that $u \in Ker\, T_u(t)$ and we get that $(Ran\,(T_u(t))^*)^\perp \subseteq Ker\, T_u(t)$.

In order to verify the validity the first equality in Eq. (30) we use the semigroup property of $\{T_u(t)\}_{t\in\mathbb{R}}$ and Eq. (32). For $t_1 \le t_2$ we get

$$\hat{P}_{t_1]}\hat{P}_{t_2]} = (I-\hat{P}_{[t_1})(I-\hat{P}_{[t_2}) = I-\hat{P}_{[t_1}-\hat{P}_{[t_2}+(T_u(t_1))^*T_u(t_1)(T_u(t_2))^*T_u(t_2) =$$
$$= I-\hat{P}_{[t_1}-\hat{P}_{[t_2}+(T_u(t_1))^*(T_u(t_2-t_1))^*T_u(t_2) = I-\hat{P}_{[t_1}-\hat{P}_{[t_2}+(T_u(t_2))^*T_u(t_2) =$$
$$= I-\hat{P}_{[t_1}-\hat{P}_{[t_2}+\hat{P}_{[t_2} = \hat{P}_{t_1]}\,.$$

We need to show also that $Ker\, T_u(t_1) \subset Ker\, T_u(t_2)$ for $t_2 > t_1$. Note that since for $t_2 > t_1$ we have $T_u(t_2) = T_u(t_2-t_1)T_u(t_1)$ and since $(T_u(t))^*$ is isometric on $\mathcal{H}^2_+(\mathbb{R})$ then it is enough to show that $Ker\, T_u(t) \neq \{0\}$ for every $t > 0$. If this condition is true and if $f \in Ker\, T_u(t_2-t_1)$ we just set $g = (T_u(t_1))^*f$ and we get that

$$T_u(t_1)g = T_u(t_1)(T_u(t_1))^*f = f$$

and

$$T_u(t_2)g = T_u(t_2)(T_u(t_1))^*f = T_u(t_2-t_1)f = 0\,.$$

In order to show that $Ker\, T_u(t) \neq \{0\}$ for every $t > 0$ we exhibit a state belonging to this kernel. Indeed one may easily check that for a complex constant μ such that $Im\,\mu < 0$ and for $t_0 > 0$ the function

$$f(\sigma) = \frac{1}{\sigma-\mu}\left[1-e^{i\sigma t_0}e^{-i\mu t_0}\right], \quad \sigma\in\mathbb{R}$$

is such that $f \in Ker\, T_u(t) \subset \mathcal{H}^2_+(\mathbb{R})$ for every $t \ge t_0 > 0$.

Finally, it is immediate that $\hat{P}_{0]} = 0$ and, moreover, since for every $f \in \mathcal{H}^2_+(\mathbb{R})$ we have $\|\hat{P}_{[t}f\|^2 = (f, \hat{P}_{[t}f) = (f, (T_u(t))^*T_u(t)f) = \|T_u(t)f\|^2$ then $s-\lim_{t\to\infty}\hat{P}_{[t} = 0$ and hence $s-\lim_{t\to\infty}\hat{P}_{t]} = I_{\mathcal{H}^2_+(\mathbb{R})}$. ∎

For $t \ge 0$ define $P_{t]} := R^*\hat{P}_{t]}R$ and $P_{[t} := R^*\hat{P}_{[t}R = I_{\mathcal{H}} - P_{t]}$. Combining Theorem 1 and Eq. (28) and taking into account the unitarity of the mapping R we conclude that there exists families $\{P_{t]}\}_{t\in\mathbb{R}^+}$, $\{P_{[t}\}_{t\in\mathbb{R}^+}$, of orthogonal projections in $\mathcal{H}$ such that $P_{t]} + P[t = I_{\mathcal{H}}$ and

$$Ran\, P_{t]} = Ker\, Z(t), \quad Ran\, P_{[t} = (Ker\, Z(t))^{\perp}, \quad t \ge 0\,,$$
$$P_{t]} = [Z(t), Z^*(t)], \quad t \ge 0\,,$$
$$P_{[t} = Z^*(t)Z(t), \quad t \ge 0\,,$$
$$P_{t_1]}P_{t_2]} = P_{t_1]}, \quad t_2 \ge t_1 \ge 0, \qquad Ran\, P_{t_1]} \subset Ran\, P_{t_2]}, \quad t_2 > t_1 \tag{33}$$

and

$$P_{0]} = 0, \qquad \lim_{t\to\infty} P_{t]} = I_{\mathcal{H}}\,. \tag{34}$$

In addition we have

$$Ran\,(Z^*(t)) = (Ker\, Z(t))^{\perp}$$

and

$$Z(t)Z^*(t) = I_{\mathcal{H}}, \quad t \ge 0\,.$$

Eqns. (33), (34) imply that it is possible to construct from the family $\{P_{t]}\}_{t\in\mathbb{R}^+}$ of orthogonal projections a spectral family of a corresponding self-adjoint operator. First define for intervals

$$\mu_T(A) = \begin{cases} P_{b]} - P_{a]}, & A = (a,b]\,. \\ P_{b]} - P_{(a-0^+)]}, & A = [a,b]\,, \\ P_{(b-0^+)]} - P_{a]}, & A = (a,b)\,, \\ P_{(b-0^+)]} - P_{(a-0^+)]}, & A = [a,b)\,, \end{cases}$$

where $b > a > 0$ (and with $P_{(a-0^+)]}$ replaced by $P_{0]}$ for $a = 0$), and then extend μ_T to the Borel σ-algebra of $\mathbb{R}^+$. Following the definition of the spectral measure $\mu_T : \mathcal{B}(\mathcal{H}) \mapsto \mathcal{P}(\mathcal{H})$ we subsequently are able to define a self-adjoint operator $T : \mathcal{D}(T) \mapsto \mathcal{H}$ via

$$T := \int_0^\infty t\, d\mu_T(t)\,.$$

By construction it is immediate that T has the properties listed in Theorem 3. For example, we have

$$\mu([0,t])\mathcal{H} = (P_{t]} - P_{0]})\mathcal{H} = P_{t]}\mathcal{H} = [Z^*(t), Z(t)]\mathcal{H}$$

and

$$\mu([t,\infty)\mathcal{H} = \lim_{t'\to\infty}(P_{t']} - P_{t]})\mathcal{H} = (I_{\mathcal{H}} - P_{t]})\mathcal{H} = P_{[t}\mathcal{H} = Z^*(t)Z(t)\mathcal{H}\,.$$

■

This concludes the proofs of the three main results of this paper.

4 Summary

The Misra, Prigogine and Courbage theory of classical and quantum microscopic irreversibility is based on the notion of Lyapounov variables. It is known from the Poincare'-Misra theorem that in the classical theory Lyapounov variables corresponding to non-equilibrium entropy cannot be associated with phase-space functions. In fact, it was shown by Misra that in Koopman's Hilbert space formulation of classical mechanics an operator corresponding to a Lyapounov variable cannot commute with all of the operators of multiplication by phase space functions. In quantum theory it was shown by Misra, Prigogine and Courbage that under assumptions (i)-(v) in Section 1 there does not exist a Lyapounov variable as an operator in the Hilbert space $\mathcal{H}$ corresponding to the given quantum mechanical problem. The solution to this problem found by Misra, Prigogine and Courbage is to turn to the Liouvillian representation of quantum mechanics and define the Lyapounov variable as a super operator on the space of density matrices. Then, under the assumption that the Hamiltonian H of the problem has absolutely continuous spectrum $\sigma(H) = \sigma_{ac}(H) = \mathbb{R}^+$ it is possible to carry out the program, define a Lyapounov variable as a super operator and find a non-unitary Λ-transformation to an irreversible representaion of the quantum dynamics.

In the present paper it is shown that if one relaxes conditions (i)-(v) in Section 1 then, under the same assumptions on the spectrum of the Hamiltonian made by Misra, Prigogine and Courbage, it is possible to construct a Lyapounov variable for the original Schrödinger evolution $U(t) = \exp(-iHt)$, $t \geq 0$ as an operator in the Hilbert space $\mathcal{H}$ of the given quantum mechanical problem without resorting to work in Liouville space and defining a Lyapounov variable as a super operator acting on density matrices. The method of proof of the existence of a Lyapounov variable is constructive and an explicit expression for such an operator is given in the form of Eq. (7). Moreover, it is shown that a Λ-transformation to an irreversible representation of the dynamics can be defined also in this case. Finally, it is demonstrated that the irreversible representation of the dynamics is the natural representation of the flow of time in the system in the sense that there exists a positive, semibounded operator T in $\mathcal{H}$ such that if μ_T is the spectral projection valued measure of T then for each $t \geq 0$ the spectral projections $P_{t]} = \mu_T([0,t))$ and $P_{[t} = (I_{\mathcal{H}} - P_{t]}) = \mu_T([t,\infty))$ split the Hilbert space $\mathcal{H}$ into the direct sum of a past subspace $\mathcal{H}_{t]}$ and a future subspace $\mathcal{H}_{[t}$

$$\mathcal{H} = \mathcal{H}_{t]} \oplus \mathcal{H}_{[t}, \quad \mathcal{H}_{t]} = P_{t]}\mathcal{H}, \quad \mathcal{H}_{[t} = P_{[t}\mathcal{H}, \quad t \geq 0$$

such that, as its name suggests, the past subspace $\mathcal{H}_{t]}$ at time $t \geq 0$ does not enter into the calculation of any matrix element of any observable for all times $t' > t \geq 0$, i.e., at time t it already belongs to the past. Put differently, in the irreversible representation the operator T provides us with a super selection rule separating past and future as there is no observable for the system that can connect the past subspace to the future subspace and all matrix elements and expectation values for $t' > t > 0$ are, in fact, calculated in the future subspace $\mathcal{H}_{[t}$.

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