QUANTUM DYNAMICAL MAPS AND RETURN TO EQUILIBRIUM*

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Let $(\mathcal{A}, \{T_t\}, \omega)$ be a dynamical system. Assume the detailed balance condition for $(\{T_t\}, \omega)$. We prove, under the new form of the spectral condition, the property of return to equilibrium for the considered dynamical system.

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1. Introduction

Let $\mathcal{A}$ be a C^*-algebra with identity, and let $T_t : \mathcal{A} \to \mathcal{A}$ be a semigroup of linear stochastic maps. Thus, T_t obeys

(i) T_t is positive: $T_t(A^*A) \geq 0$ for all $A \in \mathcal{A}$.

(ii) $T_t(1) = 1$.

(iii) $T_s \circ T_t = T_{s+t}, \qquad t, s \geq 0$.

Moreover, we shall consider, for simplicity, the uniformly continuous dynamical semigroup T_t. In nonequilibrium, isothermal quantum statistical mechanics we have usually a faithful state ω. Thus it is natural to consider the following dynamical system $(\mathcal{A}, \{T_t\}, \omega)$. We assume $(\{T_t\}, \omega)$ satisfies detailed balance condition (we denote it briefly by DBC). It involves the concept of microscopic reversibility, which was expressed in the following way: there exists an anti-linear Jordan automorphism σ of $\mathcal{A}$ of order two (that is, $\sigma^2 = \mathrm{id}$) such that

$$\omega(\sigma(A)\sigma(B)) = \omega(\sigma(AB)), \qquad \text{for } A, B \in \mathcal{A}, \tag{1}$$

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and

$$\omega(A^*B) = \omega\left(\sigma(B^*)\sigma(A)\right). \tag{2}$$

Then we say that a stochastic map on $\mathcal{A}$ obeys detailed balance if for all $A, B \in \mathcal{A}$ we have

$$\omega\left(A^*T(B)\right) = \omega\left(\sigma(B^*)T(\sigma(A))\right), \tag{3}$$

for details see [8–11].

We remind that DBC implies time invariance of the state ω, *i.e.*, $\omega \circ T_t(\cdot) = \omega(\cdot)$.

The Gelfand–Naimark–Segal construction then gives a representation π_ω of $\mathcal{A}$ on a Hilbert space $\mathcal{H}_\omega$, with cyclic vector Ω_ω, such that $\langle \Omega_\omega, \pi_\omega(A)\Omega_\omega\rangle = \omega(A)$. The action of T_t on $\mathcal{A}$ induces an action on the dense set $\pi_\omega(\mathcal{A})\Omega_\omega \subseteq \mathcal{H}_\omega$, which we denote by $\pi_\omega(T_t)$ and which is defined by

$$\pi_\omega(T_t)\pi_\omega(A)\Omega_\omega = \pi_\omega(T_tA)\Omega_\omega. \tag{4}$$

Under the above assumptions $\pi_\omega(T_t)$ is a one parameter semigroup of contractions (*cf.* [9, 11]). The aim of this note is to discuss, for a large class of dynamical systems, the interplay between spectral properties of the infinitesimal generator of $\{T_t\}$ and the return to equilibrium. It is worth pointing out that our arguments are based on the theory of $\mathcal{J}$-self-adjoint maps. Finally, some illustrative examples of $\mathcal{J}$-symmetric maps will be given in Section 3.

2. Spectral properties and return to equilibrium

Let us consider a system $(\mathcal{A}, T_t, \omega)$ satisfying DBC. As, by our assumption T_t is uniformly continuous dynamical semigroup, T_t induces on the Hilbert space of Gelfand-Segal construction $\mathcal{H}_\omega$ the uniformly continuous, $\mathcal{J}$-selfadjoint semigroup $T_t^\omega \equiv \pi_\omega(T_t)$, *i.e.* $(T_t^\omega)^* = \mathcal{J}T_t^\omega\mathcal{J}$ where $\mathcal{J}$ is the following anti-linear conjugation

$$\mathcal{J}\pi_\omega(A)\Omega_\omega = \pi_\omega(\sigma(A))\Omega_\omega\,. \tag{5}$$

Let us recall (*cf.* [5]) that a $\mathcal{J}$-selfadjoint operator has the empty residual spectrum. Let A be the infinitesimal generator of T_t^ω. We consider $\lambda \in \sigma_a(A)$, where $\sigma_a(A)$ is the approximate spectrum of A, (*cf.* [2]), *i.e.* $\lambda \in \sigma_a(A)$ iff there exits a sequence

$$\{\psi_n\} \subset \mathcal{H}_\omega \quad \text{such} \quad \text{that} \quad \|(\lambda - A)\psi_n\| \to 0. \tag{6}$$

We emphasize that although (6) *is very similar to the Weyl criterion for selfadjoint operators we are dealing with infinitesimal generators of dynamical semigroups, so, in general, with closed operators.*

We say that λ is a point in the normal approximate spectrum of A, $\lambda \in \sigma_a^n(A)$, if there exists a sequence $\{\psi_n\} \subset \mathcal{H}$ such that

$$\|(\lambda - A)\psi_n\| \to 0 \quad \text{and} \quad \|(\lambda - A)^*\psi_n\| \to 0. \tag{7}$$

Observation 1 *Let A be the infinitesimal generator of T_t and let us assume that λ is in $\sigma_a(A) \cap i\boldsymbol{R}$. Then $\lambda \in \sigma_a^n(A)$.*

Proof: Put $-B \equiv \mathrm{Re}\, A = \frac{1}{2}(A^* + A)$. The condition of dissipativeness of A implies $(x, Bx) \geq 0$ for each $x \in \mathcal{H}$. Moreover,

$$\mathrm{Re}\, A_{\lambda_0} \equiv \mathrm{Re}\,(A - i\lambda_0) = \tfrac{1}{2}(A + A^*)$$

for $\lambda_0 \in \boldsymbol{R}$. The assumption of Observation 1 implies

$$|(A_\lambda \psi_n, \psi_n)| \leq \|A_\lambda \psi_n\| \to 0$$

Consequently,

$$(\mathrm{Re}\, A_\lambda \psi_n, \psi_n) \to 0$$

as $n \to \infty$. Let E be the positive square-root of $-\mathrm{Re}\, A_\lambda$. Then

$$\|E\psi_n\|^2 = (E^2\psi_n, \psi_n) = -(\mathrm{Re}\, A_\lambda \psi_n, \psi_n) \to 0$$

as $n \to \infty$. Therefore,

$$\|\mathrm{Re}\, A_\lambda \psi_n\| = \|E^2\psi_n\| \leq \|E\|\|E\psi_n\| \to 0.$$

Finally, let us remark

$$\|A_\lambda^* \psi_n\| = \|(A_\lambda^* + A_\lambda)\psi_n - A_\lambda \psi_n\|$$

$$\leq \|(A_\lambda^* + A_\lambda)\psi_n\| + \|A_\lambda \psi_n\| \to 0\,.$$

$\diamondsuit$

Similar properties of normal approximate spectrum are described in [3]. Let us write A in the form

$$A = iH - D\,, \tag{8}$$

i.e. A is the sum of the Hamiltonian and the dissipative parts.

Remark 2 *In general, under DBC, Raggio ([13]) proved that the generator $\mathcal{L}$ of T_t is of the form $\mathcal{L} = \delta + \Psi$ where δ is the generator of one parameter group of $*$-automorphism while Ψ is the generator of the uniform continuous semigroup. Thus, the decomposition (8) is a genuine property of the considered class of dynamical systems.*

Observation 3 *Let us assume that $i\lambda \in \sigma_a^n(A) \cap i\boldsymbol{R}$. Then $\lambda \in \sigma_a(A - \gamma D)$, where γ is a real parameter, i.e. $\sigma_a(A) \cap i\boldsymbol{R}$ exhibits the stability with respect to perturbations by D.*

Proof: Let us take $\{\psi_n\}$ as in (7) and let us note that for $\alpha, \beta \in \boldsymbol{R}$,

$$\|[i(\alpha-\beta)H-(\alpha+\beta)D-i(\alpha-\beta)\lambda]\psi_n\| = \|\alpha(A-i\lambda)\psi_n+\beta(A-i\lambda)^*\psi_n\| \quad (9)$$

$$\leq |\alpha|\|(A - i\lambda)\psi_n\| + |\beta|\|(A - i\lambda)^*\psi_n\| \to 0 \quad (10)$$

In particular, for $\alpha \neq \beta$

$$\|(A - \frac{2\beta}{\alpha - \beta}D - i\lambda)\psi_n\| \to 0 \,.$$

Consequently, for $\gamma = \frac{2\beta}{\alpha-\beta}$, the Observation follows.

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Observation 4 *Let us assume $i\lambda \in \sigma_a^n(A)$. Then $0 \in \sigma_a(D)$.*

Proof:

$$2\|D\psi_n\| = \|(iH - D - i\lambda - iH - D + i\lambda)\psi_n\|$$
$$\leq \|(A - i\lambda)\psi_n\| + \|(A - i\lambda)^*\psi_n\| \to 0 \,.$$

◊

Theorem 5 *The following conditions are equivalent: (i) $i\lambda \in \sigma_a(A) \cap i\boldsymbol{R}$, (ii) $\lambda \in \sigma_a(H)$ and $0 \in \sigma_a(D)$ with the possibility of choice of the same sequence $\{\psi_n\}$ for 0 and given λ.*

Proof: $\Rightarrow$ It is enough to apply Observations 1, 3 and 4. $\Leftarrow$ Let us observe

$$\|(i\lambda - A)\psi_n\| = \|(i\lambda - iH)\psi_n + (-D)\psi_n\|$$
$$\leq \|(\lambda - H)\psi_n\| + \|D\psi_n\| \to 0 \,.$$

◊

Denote by $\mathcal{N}_a(D)$ the set of all sequences $\{\psi_n\}$, with $\psi_n \in \mathcal{H}$ ($n = 1, 2, ...$), such that $\|\psi_n\| = 1$, $\|D\psi_n\| \to 0$. In what follows, $\mathcal{N}_a(D)$ will be called the approximate kernel of D. Let $\mathcal{H}_a(H)$ denote the set of all approximate eigenvectors of the Hamiltonian part H of A corresponding to 0, *i.e.*, the set of all sequences $\{\psi_n\} \in \mathcal{H}$, ($\|\psi_n\| = 1$) such that $\|H\psi_n\| \to 0$.

Definition 6 *Spectral Condition*

$$\mathcal{N}_a(D) \subseteq \mathcal{H}_a(H)\,. \tag{11}$$

Corollary 7 *Let T_t be $\mathcal{J}$-selfadjoint, completely non unitary, uniformly continuous semigroup of contractions on a Hilbert space $\mathcal{H}$, with generator A. Let us assume the Spectral Condition. Then, $\sigma(A) \cap i\boldsymbol{R}$ is equal to $\{0\}$.*

Proof: Let $i\lambda_0$ be in $\sigma(A) \cap i\boldsymbol{R}$. Then the assumptions of Corollary imply that $i\lambda_0 \in \sigma_a(A) \cap i\boldsymbol{R}$. On the other hand, an application of Theorem 5 gives $\lambda_0 \in \sigma_a(H)$ where H is the Hamiltonian part of A. Then an application of the Spectral Condition and Theorem 5 completes the proof of Theorem. $\diamondsuit$

We shall need

Definition 8 *The semigroup V_t on $\mathcal{H}$ is strongly stable if as $t \to \infty$ $\|V_t f\| \to 0$ for all $f \in \mathcal{H}$.*

Let us recall (*cf.* [6])

Theorem 9 *Let the semigroup V_t be a contraction semigroup on $\mathcal{H}$. $\mathcal{H}$ has a maximal closed subspace $\mathcal{H}_1$ on which V_t is (i.e. restricts to) a unitary semigroup. The restriction of V_t on $\mathcal{H}_1^{\perp}$ is a completely non unitary semigroup. Moreover, both V_t and V_t^* are strongly stable on $\mathcal{H}_1^{\perp}$ if and only if $P = Q$ is a projection, where*

$$Pf = \lim_{t\to+\infty} V_t^* V_t f = \lim_{t\to+\infty} V_t V_t^* f = Qf \tag{12}$$

for $f \in \mathcal{H}$. The range of $P = Q$ is then $\mathcal{H}_1$.

Remarks 10

(i) The limits in (12) exist (cf. [4]).

(ii) A condition leading to a semigroup strongly stable on $\mathcal{H}_1^{\perp}$ was also studied in ([10]).

Theorem 11 *(see [1]) Let V_t be a bounded C_0-semigroup with generator A. Assume that $\sigma_r(A) \cap i\boldsymbol{R} = \emptyset$, where $\sigma_r(A)$ denotes the residual part of the spectrum of A. If $\sigma(A) \cap i\boldsymbol{R}$ is countable, then V_t is strongly stable C_0-semigroup.*

Theorems 9, 11 and Corollary 7 yield:

Corollary 12 *Let T_t^ω be a $\mathcal{J}$-selfadjoint, uniformly continuous semigroup of contractions on a Hilbert space $\mathcal{H}_\omega$, with generator A. Denote by $A^\perp$ the infinitesimal generator of the restriction of T_t^ω on $\mathcal{H}_1^\perp$. Let us assume the Spectral Condition for $A^\perp$. Then, $\lim_{t\to\infty}(T_t^\omega)^* T_t^\omega$ is equal to an orthogonal projection.*

Note that we have actually proved that under the assumption of DBC and the spectral condition the system $(\mathcal{M}, \pi_\omega(T_t), \omega)$, where $\pi_\omega(T_t)$ is a completely positive semigroup on the W^*-algebra $\mathcal{M} \equiv (\pi_\omega(\mathcal{A}))'' \subset \mathcal{B}(\mathcal{H}_\omega)$, shows signs of return to equilibrium. This can be rephrased as follows. Let us assume DBC and the spectral condition. Additionally let us assume the complete positivity of dynamical semigroup. Then the limit

$$\varphi_+(A) = \lim_{t\to+\infty} \varphi(\pi_\omega(T_t)(A)) \tag{13}$$

exists for $A \in \mathcal{M}$ and normal states φ provided that $\lim_{t\to+\infty} \omega(A\pi_\omega(T_t)(B))$ exists for all A in a σ-weakly subset of $\mathcal{M}$ and B in the largest $\pi_\omega(T)$-invariant W^*-subalgebra $\mathcal{N}$ on which $\pi_\omega(T_t)$ is equal to a group of automorphisms. The assumption of complete positivity is necessary for a characterization of $\mathcal{N}$ (*cf.* [12]). The equality (13) may be proved in much same way as Theorem in ([10]) with the spectral condition taking the place of the asymptotic normality assumption. In other words, *as the spectral condition can be considered as being more intrinsic property of dynamical system we got the strengthening of the description of return to equilibrium.*

3. Examples

In the previous section it was indicated how analysis of $\mathcal{J}$-symmetric maps can be used for a study of the question concerning the return to equilibrium. Now, we want to show that $\mathcal{J}$-symmetricity arise naturally, also, in the elementary Quantum Mechanics. Let $\mathcal{H} \equiv L_2(\boldsymbol{R}^n)$ be a Hilbert space associated with a quantum system. On that Hilbert space we consider the Schrödinger operator S with complex-valued potential $V = V_1 + iV_2$, V_1, V_2 real-valued, measurable functions, *i.e.* $S \equiv \Delta + V$. Then one can show that S is a $\mathcal{J}$-self-adjoint operator (*cf.* [5]), where (in that case) the conjugation $\mathcal{J}$ on $\mathcal{H}$ is induced by the complex conjugation on $\boldsymbol{C}$. It is obvious, that under the assumption $V_2 \geq 0$, iS generates a semigroup on $\mathcal{H}$. To get an interesting example of a class of operators satisfying conditions of the previous section we recall: Let V_2 be a bounded real-valued function on a measure space (Y, μ); $Y \subseteq \boldsymbol{R}^n$. Define

$$(T_{V_2} g)(y) = V_2(y) g(y), \quad g \in L_2(Y, \mu). \tag{14}$$

Then, $\sigma(T_{V_2})$ is equal to the essential range of V_2. Suppose additionally that V_2 is continuously differentiable, $\operatorname{grad} V_2 \neq 0$ almost everywhere in Y, then T_{V_2} is spectrally absolutely continuous (*cf.* [7]). Moreover, let V_1 be a locally bounded, positive function such that $V_1(y) \to \infty$ for $|y| \to \infty$. The important point to note here is that the just considered class of functions contains potentials of oscillators (harmonic, anharmonic, *etc.*) Then $-\Delta + V_1 \equiv H$ (the sum is taken in the sense of quadratic forms) has only discrete spectrum (*cf.* [14]). Clearly, to have a concrete example of such the sum one can take H to be the Hamiltonian operator associated with a model of oscillator.

To illustrate the main idea of our analysis let us consider, as an example, one dimensional oscillator. Thus, H is taken to be $H = \frac{1}{2}(-\frac{d^2}{dx^2} + x^2)$. One can verify that H is a selfadjoint operator, $\sigma(H)$ is pure discrete, and $\mathcal{H}_a(H) = \emptyset$. Further, let us take as a dissipative perturbation D of H that given by T_{V_2}. We remind that to get a well defined semigroup we have to assume $V_2 \geq 0$. Let us apply Theorem 5 and its corollaries to the pair $(iH, -D)$. To this end we assume that $i\lambda \in \sigma_a(iH - D) \cap i\boldsymbol{R}$. Theorem 5 implies that $\lambda \in \sigma(H)$ and $0 \in \sigma(D)$ with the same choice of vectors $\{\psi_n\}$. But the spectrum of H is pure discrete, it does not contain 0, the spectrum of D is pure continuous so (*ii*) of Theorem 5 does not hold. Consequently $i\lambda \notin \sigma_a(iH - D) \cap i\boldsymbol{R}$ and, for example, Theorem 11 implies the strong stability of the semigroup $V_t = \exp\{iHt - Dt\}$. On the other hand, if we consider a slightly shifted Hamiltonian part $H' = H - \frac{1}{2}\mathbf{1}$ then $\sigma(H')$ is pure discrete, it contains 0, $\sigma(D)$ is pure continuous, it can contain 0 (with a suitable choice of the function V_2) and therefore the pair $(iH', -D)$ provides a nice example where the spectral condition is useful.

To conclude this brief discussion one may say that the presented simple models clearly indicate that the spectral condition presenting some compatibility requirement between fixed points of dissipation and invariant states of Hamiltonian part of dynamics can be also useful in concrete models of Quantum Mechanics.

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