AN ALGEBRAIC CONDITION FOR THE APPROACH TO EQUILIBRIUM OF AN OPEN N-LEVEL SYSTEM

HERBERT SPOHN
Fachbereich Physik der Ludwig-Maximilians-Universität München, Germany

ABSTRACT. We give an algebraic condition in order that a completely positive dynamical semigroup of an N-level system has a unique (invariant) equilibrium state and that every initial state approaches this equilibrium state as $t \to \infty$. We apply our result to a semigroup arising in the weak coupling limit.

1. INTRODUCTION

The time evolution of a small quantum system of finitely many degrees of freedom coupled to infinite quantum systems, called reservoirs, can be described, under certain limiting conditions, by a one-parameter semigroup of transformations [1, 2, 3, 4]. Let $\mathcal{H}$ be the Hilbert space of the small system with dim $(\mathcal{H}) = N$ and let $\Lambda_t : B(\mathcal{H}) \to B(\mathcal{H})$, $t \in R^+$, be the dynamical semigroup, where $B(\mathcal{H})$ is the C^*-algebra of all bounded operators on $\mathcal{H}$. It is assumed that (1) Λ_t is linear, (2) Λ_t is trace preserving, (3) the dual map Λ_t^* is completely positive, (4) $\Lambda_t\Lambda_s = \Lambda_{t+s}$, $s, t \geqslant 0$, and (5) $\lim_{t\to 0} \Lambda_t = 1$. Then by the Hille-Yosida theorem $\Lambda_t = e^{Lt}$ and it can be shown that $\|\Lambda_t\| = 1$. According to [5, 6] the generator $L:B(\mathcal{H}) \to B(\mathcal{H})$ of such a completely positive dynamical semigroup on $B(\mathcal{H})$ has the form

$$L: \rho \mapsto L(\rho) = -i[H, \rho] + \frac{1}{2} \sum_{j\in I} ([V_j, \rho V_j^*] + [V_j\rho, V_j^*]) \tag{1}$$

with $H = H^* \in B(\mathcal{H})$, $V_j \in B(\mathcal{H})$, $\sum_{j\in I} V_j^* V_j \in B(\mathcal{H})$.

A question of obvious physical interest is to give a condition for the V_j's such that the semigroup $\{e^{Lt} | t \in R^+\}$ has a unique invariant state (= equilibrium state) and such that every initial state tends to this equilibrium state as $t \to \infty$. A semigroup with this property will be called *relaxing.* In this paper we derive a simple algebraic condition for a dynamical semigroup to be relaxing. In the microscopic picture the V_j's arise from the interaction with the reservoirs. If there is a good coupling between the small system and the reservoirs, then the reservoirs should drive the small system into equilibrium (i.e. either thermodynamic equilibrium, if the reservoirs have the same temperature, or steady state, if the reservoir temperatures are different). Therefore our algebraic condition should imply a condition for the interaction term to give rise to an *effective*

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coupling. In Section 3 we will derive such a condition for a semigroup arising in the weak coupling limit [1].

2. THE ALGEBRAIC CONDITION

DEFINITION 1. *The dynamical semigroup* $\{\Lambda_t = e^{Lt} | t \in R^+\}$ *on* $B(\mathcal{H})$ *with* L *given by* (1) *is called relaxing, if there exists a state* $\rho_0 \in B(\mathcal{H})$ *such that for every state* $\rho \in B(\mathcal{H})$

$$\lim_{t\to\infty} \Lambda_t(\rho) = \rho_0 . \tag{2}$$

Davies [7] has shown that, if no proper subspace of $\mathcal{H}$ is invariant under all V_j, $j \in I$, then the semigroup $\{\Lambda_t = e^{Lt} | t \in R^+\}$ is relaxing. If $1sp\ \{V_j | j \in I\}$ is self-adjoint, then we arrive at the following algebraic condition ($'$ denotes the commutant in $B(\mathcal{H})$):

THEOREM 2. *Let* $L{:}B(\mathcal{H}) \to B(\mathcal{H})$ *be given by* (1). *If* $1sp\ \{V_j | j \in I\}$ *is self-adjoint and if* $\{V_j | j \in I\}'' = B(\mathcal{H})$, *then the semigroup* $\{\Lambda_t = e^{Lt} | t \in R^+\}$ *is relaxing.*

Proof. We want to present here a proof, completely different from the one in [7], which is based on the spectral properties of L.

Let $B(\mathcal{H})$ be equipped with the scalar product $\mathrm{tr}(A^*B)$. Since $\mathcal{K} = 1sp\ \{V_j, 1 | j \in I\}$ is self-adjoint, we can choose a self-adjoint basis $\left\{F_1, \ldots, F_p, \frac{1}{\sqrt{N}} 1\right\}$ in $\mathcal{K}$. Expanding

$$V_j = \sum_{m=1}^{p} v_{jm} F_m + v_j 1 \tag{3}$$

we obtain

$$L(\rho) = -i[H + \overline{H}, \rho] + \frac{1}{2} \sum_{m,n=1}^{p} b_{mn} ([F_m, \rho F_n] + [F_m \rho, F_n]). \tag{4}$$

By construction, the matrix $b_{mn} = \sum_{j\in I} v_{jm} v_{jn}^*$ is strictly positive. Let $\alpha > 0$ be smaller than its smallest eigenvalue and let $L = L_1 + L_2$ be such that

$$L_2(\rho) = \frac{\alpha}{2} \sum_{m=1}^{p} ([F_m, \rho F_m] + [F_m \rho, F_m]) \tag{5}$$

It follows from [6, Theorem 2.2] that L_1 is the generator of a completely positive dynamical semigroup and that, consequently, L_1 is dissipative. We easily compute

$$\mathrm{tr}(\rho^* L_2(\rho)) = -\frac{\alpha}{2} \sum_{m=1}^{p} \mathrm{tr}(([F_m, \rho])^*) ([F_m, \rho])) \leqslant 0. \tag{6}$$

By presupposition $\{V_j | j \in I\}' = \{C1\}$, which implies $\{F_m | m = 1, \ldots, p\}' = \{C1\}$. Now

$\mathrm{tr}(\rho^* L_2(\rho)) = 0$ implies $[F_m, \rho] = 0$ for $m = 1, ..., p$ and therefore $\rho = c1$. Let $\tilde{L}, \tilde{L}_1, \tilde{L}_2$ denote the projection of L, L_1, L_2 on $B(\mathcal{H}) \ominus \{C1\}$.

($\tilde{L}, \tilde{L}_1, \tilde{L}_2$ are operators on $B(\mathcal{H}) \ominus \{C1\}$.) From the foregoing we conclude that the spectrum of $\tilde{L}_2$ lies in the open left hand real axis. The characteristic equation of L_1 shows that $\tilde{L}_1$ has one eigenvalue zero less than L_1 (counted by their algebraic multiplicity). Therefore $\|e^{\tilde{L}_1 t}\|_1 \leqslant 1$ where $\|\cdot\|_1$ denotes the norm restricted to $B(\mathcal{H}) \ominus \{C1\}$. Since $\{e^{\tilde{L}_2 t} | t \in R^+\}$ is a strictly contracting semigroup, it follows from the Trotter product formula that $\|\exp(\tilde{L}_1 + \tilde{L}_1)t\|_2 \leqslant e^{-\lambda t}$ for all $t \in R^+$ with $\lambda > 0$. Therefore all eigenvalues of $\tilde{L}$ lie in the open left hand complex plane. The characteristic equation of L shows that the spectrum of L is the spectrum of $\tilde{L}$ with exactly one eigenvalue zero added. This proves the theorem. ∎

Remark. For semigroups given in the form of [6] we proved in [8] a sufficient condition for relaxing unrelated to the present one.

3. AN APPLICATION

Davies [1] considers an N-level system weakly coupled to an infinite free heat reservoir with inverse temperature β. The coupling has the form $Q \otimes \Phi$, where $Q = Q^* \in B(\mathcal{H})$ and the self-adjoint operator Φ is a suitable combination of field operators of the reservoir. In the weak coupling limit he obtains a dynamical semigroup $\{e^{Kt} | t \in R^+\}$, where K is of the form (1). Let $H = H^* \in B(\mathcal{H})$ be the Hamiltonian of the uncoupled N-level system with eigenvalues λ_k and spectral projections P_k, $k = 1, ..., M$. Then the V_j's occuring in (1) are in this case the $\sqrt{\hat{h}(\omega)}\, A_\omega$'s, where ω varies over the spectrum $\sigma([H, \cdot])$ of the Liouville-von Neumann operator $[H, \cdot]$. We have $\hat{h}(-\omega) = e^{-\beta\omega}\hat{h}(\omega) \geqslant 0$ and $A_\omega = \Sigma P_k Q P_j$, where the sum is taken such that $\lambda_k - \lambda_j = \omega \in \sigma([H, \cdot])$. Applying Theorem 2 to the present situation we obtain

THEOREM 3. *Let K be as introduced above. If $\hat{h}(\omega) > 0$ for all $\omega \in \sigma([H, \cdot])$ and if $\{H, Q\}'' = B(\mathcal{H})$, then the dynamical semigroup $\{e^{Kt} | t \in R^+\}$ is relaxing. The unique equilibrium state is the canonical ensemble $e^{-\beta H}/\mathrm{tr}(e^{-\beta H})$.*

Proof. Let $U(t) = e^{iHt}$. First, we show that $\{H, Q\}'' = B(\mathcal{H})$ implies $\{U(t)QU(t)^* | t \in R\}'' = B(\mathcal{H})$. (Choosing $Q = 1$ shows that, in general, one has only a proper inclusion.)

(i) Let $A_j \in B(\mathcal{H})$, $j = 1, ..., m$, $\lambda_j \in R$, $\lambda_j \neq \lambda_k$ and let

$$\sum_{j=1}^{m} e^{i\lambda_j t} A_j = 0$$

for all $t \in R$. Since the $1sp\ \{(e^{i\lambda_1 t}, ..., e^{i\lambda_m t}) | t \in R\}$ is the whole m-dimensional linear space, we conclude that $A_j = 0$ for $j = 1, ..., m$.

(ii) Let the eigenvalues $\{\lambda_j | j = 1, ..., M\}$ of H be ordered increasingly with increasing j and let P_j be the corresponding spectral projections. Let $P \in \{U(t)QU(t)^* | t \in R\}'$. Since $Q = Q^*$, we can assume, without loss of generality, that $P = P^*$. Then $[U(t)QU(t)^*, P] = 0$ implies

$$\sum_{j=1}^{m} e^{i(\lambda_1 - \lambda_j)t} P_1 Q P_j P P_1 - \sum_{k=1}^{M} e^{i(\lambda_k - \lambda_1)t} P_1 P P_k Q P_1 = 0 \tag{7}$$

for all $t \in R$. Since $\lambda_1 - \lambda_j \leqslant 0$ and $\lambda_k - \lambda_1 \geqslant 0$ with equality only if $j = 1 = k$, we can conclude from (i)

$$\begin{aligned} &P_1 Q P_j P P_1 = 0 \quad \text{for} \quad j \neq 1, \\ &P_1 Q P_1 P P_1 = P_1 P P_1 Q P_1. \end{aligned} \tag{8}$$

Furthermore, $[U(t)QU(s)QU(s+t)^*, P] = 0$ implies

$$\begin{aligned} &\sum_{j=1}^{M} e^{i(\lambda_1 - \lambda_j)t} e^{-i\lambda_j s} P_1 Q U(s) Q P_j P P_1 \\ &- \sum_{k=1}^{M} e^{i(\lambda_k - \lambda_1)t} e^{-i\lambda_1 s} P_1 P P_k Q U(s) Q P_1 = 0 \end{aligned} \tag{9}$$

for all $s, t \in R$. As above we conclude $P_1 Q U(s) Q P_j P P_1 = 0$ for $j \neq 1$ and $P_1 Q U(s) Q P_1 P P_1 = P_1 P P_1 Q U(s) Q P_1$ for all $s \in R$. Continuing this procedure we obtain

$$P_1 Q U(t_1) Q \ldots Q U(t_n) Q P_j P P_1 = 0 \quad \text{for} \quad j \neq 1 \tag{10}$$

$$P_1 Q U(t_1) Q \ldots Q U(t_n) Q P_1 P P_1 = P_1 P P_1 Q U(t_1) Q \ldots Q U(t_n) Q P_1 \tag{11}$$

for all $t_1, \ldots, t_n \in R$, $n = 1, 2, \ldots$

(iii) Since $\{H, Q\}'' = B(\mathcal{H})$, an arbitrary $A \in B(\mathcal{H})$ is a suitable linear combination of products of the form $f_1(H) g_1(Q) \ldots f_m(H) g_m(Q)$, $m = 1, 2, \ldots$, where we admit that $f_1(H) = 1$, $g_m(Q) = 1$. Then $P_1 A P_j$ is a suitable linear combination of products of the form $P_1 g_1(Q) f_2(H) \ldots f_m(H) g_m(Q) P_j$. Suitable linear combinations in (10) produce

$$P_1 g_1(Q) f_2(H) \ldots f_m(H) g_m(Q) P_j P P_1 = 0. \tag{12}$$

For $m = 1$ and $g_1(Q) = 1$ (12) holds trivially. Therefore $P_1 A P_j P P_1 = 0, j \neq 1$, for all $A \in B(\mathcal{H})$ which implies

$$P_j P P_1 = 0 = P_1 P P_j \tag{13}$$

for $j \neq 1$. In the case $j = 1$ suitable linear combinations in (11) produce

$$\begin{aligned} &P_1 g_1(Q) f_2(H) \ldots f_m(H) g_m(Q) P_1 P P_1 \\ &= P_1 P P_1 g_1(Q) f_2(H) \ldots f_m(H) g_m(Q) P_1. \end{aligned} \tag{14}$$

For $m = 1$ and $g_1(Q) = 1$ (14) holds trivially. Therefore $P_1AP_1PP_1 = P_1PP_1AP_1$ for all $A \in B(\mathcal{H})$ which implies

$$P_1PP_1 = \alpha_1 P_1, \qquad \alpha_1 \in R. \tag{15}$$

(iv) $[U(t)QU(t)^*, P] = 0$ implies

$$\sum_{j=1}^{M} e^{i(\lambda_2 - \lambda_j)t} P_2QP_jPP_2 - \sum_{k=1}^{M} e^{i(\lambda_k - \lambda_2)t} P_2PP_kQP_2 = 0 \tag{16}$$

for all $t \in R$. $\lambda_2 - \lambda_j = \lambda_k - \lambda_2$ only if either $j = 2 = k$ or either $j = 1$ or $k = 1$. However, in the second case, by (13), $P_1PP_2 = 0 = P_2PP_1$. Therefore we conclude from (i)

$$\begin{aligned} &P_2QP_jPP_2 = 0 \quad \text{for} \quad j \neq 2 \\ &P_2QP_2QP_2 = P_2PP_2QP_2. \end{aligned} \tag{17}$$

Going through the same steps as in (ii) and (iii) we obtain $P_2AP_jPP_2 = 0, j \neq 2$, and $P_2AP_2PP_2 = P_2PP_2AP_2$ for all $A \in B(\mathcal{H})$ which implies

$$\begin{aligned} &P_jPP_2 = 0 = P_2PP_j \quad \text{for} \quad j \neq 2 \\ &P_2PP_2 = \alpha_2 P_2, \qquad \alpha_2 \in R. \end{aligned} \tag{18}$$

By the same method we study successively $P_jPP_3, ..., P_jPP_M, j = 1, ..., M$ and we obtain $P_jPP_k = 0$ for $j \neq k$ and $P_jPP_j = \alpha_j P_j$, $\alpha_j \in R, j,$ $k = 1, ..., M$. From $[Q, P] = 0$ and $\{H, Q\}'' = B(\mathcal{H})$ we conclude that $\alpha_j = \alpha$ for $j = 1, ..., M$ and that therefore $P = \alpha 1$.

(v) We have $U(t)QU(t)^* = \sum_\omega e^{i\omega t} A_\omega$. Therefore $\{A_\omega | \omega \in \sigma([H, \cdot])\}'' = B(\mathcal{H})$ and, by Theorem 2, $\{e^{Kt} | t \in R^+\}$ is relaxing. According to [1, Theorem 4.5] the canonical ensemble $e^{-\beta H}/\mathrm{tr}(e^{-\beta H})$ is always an invariant state for $\{e^{Kt} | t \in R^+\}$. (Going through the proof, it is easy to see that this assertion is independent of the degeneracy of H.) Since the semigruop $\{e^{Kt} | t \in R^+\}$ has only one invariant state, this invariant state has to be the canonical ensemble. ■

In [1] one finds another sufficient condition for relaxation: $\hat{h}(\omega) > 0$, H has a multiplicity free spectrum and $\langle r|Q|s\rangle \neq 0$, where the $|r\rangle$'s are the eigenvectors of H. Obviously, this condition is stronger than the one given in Theorem 3.

Theorem 3 gives a physically appealing criterion for an effective coupling between the N-level system and the reservoir: $\hat{h}(\omega) > 0$ for all $\omega \in \sigma([H, \cdot])$ means that the reservoir has to be coupled at all to the relevant frequencies. $\{H, Q\}'' = B(\mathcal{H})$ tells us that, besides the unit operator, there is no other operator in $B(\mathcal{H})$ which commutes with both the Hamiltonian H and the 'interaction operator' Q, i.e. H and Q are so incompatible that they generate algebraically the whole algebra of observables $B(\mathcal{H})$.

In the case that there are several reservoirs with the same type of coupling, the generator $\bar{K}$ of the dynamical semigroup has the form $\bar{K} = \sum_{j=1}^{q} K_j$, where the K_j's are built from the operators $Q_j = Q_j^* \in B(\mathcal{H})$ in the same way as K was built from Q. The sufficient condition in Theorem 3 is then replaced by $\hat{h}_j(\omega) > 0$ for all $\omega \in \sigma([H, \cdot]), j = 1, ..., q$, and $\{H, Q_j | j = 1, ..., q\}'' = B(\mathcal{H})$. The unique equilibrium state is the canonical ensemble only if all the reservoirs have the same temperature.

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