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ON OPEN SYSTEM DYNAMICS —AN OPERATOR ALGEBRAIC STUDY—

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Abstract

The open system dynamics is rigorously studied within the C^*-algebraic framework in terms of the approach to equilibrium. It is pointed out that every combined state of every state of a finite system and an equilibrium state describing an infinite reservoir relaxes to equilibrium through an interaction between both systems when the total Hamiltonian of the combined system satisfies some spectral properties.

Sec. I: Introduction.

The approach to equilibrium of a dynamical system is one of the most important problems to be solved in quantum statistical mechanics [1, 2, 3, 4]. The principle aim of this paper is to study the problem of this type for a finite system interacting with an infinite reservoir in equilibrium.

The motivation of this work is as follows: Some physicists think that the system to be measured or in which some experiments are performed should be finite even if it is large compared with the radius of an atom. However, if a system is finite and isolated, any time dependent state of the system will not relax to equilibrium because the basic Schrödinger equation of motion is reversible under time reflection. From evidence accumulated by experiments, most of physical systems relax to some equilibrium after long time. This fact tells that we had better treat such finite system as open system, namely, interactions between the finite system and the outside of the system (the so-called reservoir) should be taken into account. We then expect that physically interesting combined states of the system and the reservoir will relax to equilibrium through an interaction between them.

In this paper, we obtain conditions under which such relaxation occurs. We here take the Kubo-Martin-Schwinger (K. M. S.) condition [5, 6, 7] as that of equilibrium of our systems considered since any Gibbs state satisfies this condition and the K. M. S. condition seems most appropriate [8, 9] to discuss thermal equilibrium in quantum statistical mechanics.

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Sec. II: Formulation of the Problems.

Let $\mathcal{H}^S$ be a Hilbert space of a system S and H^S denote a self-adjoint lower bounded Hamiltonian of S. We often call the system S finite when the volume of S is finite or the degrees of freedom of S is finite. Our system S is assumed to have finite volume, so the spectrum of H^S becomes discrete. Let our finite system S be described by a triple $(\mathcal{A}^S, \mathfrak{S}^S, \alpha_t^S)$, where $\mathcal{A}^S$ is the C^*-algebra $B(\mathcal{H}^S)$ of all bounded linear operators on the Hilbert space $\mathcal{H}^S$, $\mathcal{S}^S$ is the set of all normal states on $\mathcal{A}^S$ (i. e., the set of all linear functionals ϕ^S on $\mathcal{A}^S$ such that $\phi^S(A^*A)\geqq 0$ for any $A\in\mathcal{A}^S$, $\phi^S(I^S)=1$ for unity I^S of $\mathcal{A}^S$ and $\phi^S(A_\alpha)\uparrow\phi(A)$ for $A_\alpha\uparrow A$, filtering upwards, in $\mathcal{A}^S$), and α_t^S $(t\in\boldsymbol{R})$ is the time evolution automorphism of $\mathcal{A}^S$ generated by the Hamiltonian H^S.

On the other hand, an infinite reservoir R is described by another triple $(\mathcal{A}^R, \mathcal{S}^R, \alpha_t^R)$, where $\mathcal{A}^R$ is a C^*-algebra with unity I^R, $\mathcal{S}^R$ is the set of all states on $\mathcal{A}^R$ and α_t^R $(t\in\boldsymbol{R})$ is a strongly continuous one-parameter automorphism of $\mathcal{A}^R$. We assume that the infinite reservoir is initially in equilibrium described by a faithful K. M. S. state φ^R at the inverse temperature β with respect to α_t^R. It is said that the state φ^R satisfies the K. M. S. condition at β w. r. t. the automorphism α_t^R if for any pair A, B in $\mathcal{A}^R$, there exists a bounded function $F_{A,B}(z)$ of the complex number z holomorphic in and continuous on the strip $-\beta\leqq\mathrm{Im}\,z\leqq 0$ such that $F_{A,B}(t)=\varphi^R(\alpha_t^R(A)B)$ and $F_{A,B}(t-i)=\varphi^R(B\alpha_t^R(A))$ for any $t\in\boldsymbol{R}$. By the Gelfand-Naimark-Segal (G. N. S.) construction theorem, to the state φ^R there correspond a Hilbert space $\mathcal{H}^R$, a cyclic vector Φ^R, a representation π^R being a *-homomorphism from the C^*-algebra $\mathcal{A}^R$ to the set $B(\mathcal{H}^R)$ of all bounded linear operators on the Hilbert space $\mathcal{H}^R$ and a strongly continuous one-parameter unitary group U_t^R such that $\pi^R(\alpha_t^R(A))=U_t^R\pi^R(A)U_t^{R*}$ for any $A\in\mathcal{A}^R$ and $U_t^R\Phi^R=\Phi^R$.

Let us take any faithful state $\phi^S\in\mathcal{S}^S$ of S and consider its time development. When the system S is isolated and the state ϕ^S is not α_t^S-invariant (i. e. $\phi^S(\alpha_t^S(A))\neq\phi^S(A)$ for some $A\in\mathcal{A}^S$), the expectation value $\phi^S(\alpha_t^S(A))$ is periodic or at least almost periodic function in t because the system S is finite. Thus $\phi^S(\alpha_t^S(A))$ does not relax to equilibrium for all $A\in\mathcal{A}^S$ when time t tends to infinite. That is, the infinite time limit of $\phi^S\circ\alpha_t^S$ in the weak*-topology does not exist. We hence need to take account of the effect of an infinite reservoir on the finite system S in order to explain such relaxation behavior.

The initial (non-interacting) combined system of the system S and the reservoir R is described by the following:

(1-1) Algebra: $\mathcal{A}=\mathcal{A}^S\otimes\mathcal{A}^R$,

(1-2) State: $\phi=\phi^S\otimes\varphi^R\in\mathcal{S}=\mathcal{S}^S\otimes\mathcal{S}^R$,

(1-3) Time evolution: $\alpha_t^0=\alpha_t^S\otimes\alpha_t^R$,

(1-4) Hilbert space: $\mathcal{H}=\mathcal{H}^S\otimes\mathcal{H}^R$,

(1-5) Representation: $\pi=i^S\otimes\pi^R$ (i^S is the identity map onto $\mathcal{A}^S$).

Let us introduce an interaction between the systems S and R. The interaction will be a bounded self-adjoint element $V=V^*\in\mathcal{A}$. By Stone's theorem, there exists a self-adjoint operator H^R which generates the unitary one parameter group U_t^R, i. e., $U_t^R=\exp(iH^R t)$. We may call $H=H^S+H^R+\pi(V)$ the total Hamiltonian of the combined system, which generates the so-called perturbed time evolution automorphism α_t of $\mathcal{A}$ [10]:

$$\alpha_t(A)=\sum_{n\geq 0} i^n \int_{0\leqq t_1\leqq\cdots\leqq t_n\leqq t} dt_1\cdots\int dt_n[\alpha_{t_1}^0(V), \cdots[\alpha_{t_n}^0(V), \alpha_t^0(A)]\cdots] \tag{1-6}$$

for $t\geqq 0$ (the case $t\leqq 0$ is due to exchange of 0 and t in the above integral domain).

Considering the combined system and any faithful state on $\mathcal{A}$ denoted by $\phi=\phi^S\otimes\varphi^R$, it is natural for us to ask the following question:

"*Under what conditions on the dynamical system does the limit* $w^*-\lim_{|t|\to\infty}\phi\circ\alpha_t$ *exist and is it identical to a proper eqilibrium (K. M. S.) state at the inverse temperature* β *with respect to the automorphism* α_t?"

This problem concerns the relaxation process of the combined system. In conventional discussions of physics, one does not worry about such question but takes it for granted. By answering this question, we expect that the restriction of the limiting state to the algebra $\mathcal{A}^S$ of the system S might be close, in some sense, to the K. M. S. state of S with the same temperature of the reservoir R, and we can also explain some physical phenomena of the so-called relaxation processes; for example, if the temperature of the system is initially different from that of the reservoir, our experience tells that if the system is in contact with the reservoir, then the temperature of the system goes to that of the reservoir. We finally note that our investigation here is concerned with the time development of the combined system but not of the system itself. It is really important to study directly the time development of a state of the system under the effect of some interaction with an infinite reservoir. For this purpose, the technique of conditional expectation invented by H. Umegaki [11] will be essential. This aspect will be discussed elsewhere [12].

Sec. III: Relaxation Process.

In this section, we study the problem presented in the previous section.

As mentioned before, the initial temperature of the system S might be different from that of the reservoir R, or the initial state ϕ^S of S might not be α_t^S-invariant. In any case, there exists a trace class operator $\rho^S=\exp(-\beta H^S)/\mathrm{Tr}\exp(-\beta H^S)$ so that the state φ^S defined by $\varphi^S(A)=\mathrm{Tr}\,\rho^S A$ for any $A\in\mathcal{A}^S$ satisfies the K. M. S. condition at the inverse temperature β of the reservoir with respect to the automorphism α_t^S of the system. Thus the state $\varphi^S\otimes\varphi^R$ on $\mathcal{A}$ satisfies this condition at β w. r. t. $\alpha_t^0=\alpha_t^S\otimes\alpha_t^R$. Let us denote this state by φ in the sequel discussions. Moreover, for a faithful normal state ϕ^S on $\mathcal{A}^S$ which may not be α_t^S-invariant, we denote the combined state with the equilibrium state φ^R of the reservoir by $\phi=\phi^S\otimes\varphi^R$ as in (1-2).

Let us start by proving several lemmas.

LEMMA 1. *Let ω be a state on $\mathcal{A}$ and χ be another state on $\mathcal{A}$ dominated by ω, i.e., $\chi\leqq\lambda\omega$ for some $\lambda>0$. Then for any $\varepsilon>0$, there exists an element W in $\mathcal{A}$ such that*

$$|\chi(A)-\omega(AW)|<\varepsilon\|A\|$$

for any $A\in\mathcal{A}$.

Proof. It is well-known that for any state χ dominated by ω, there exists a positive operator B in $\pi_\omega(\mathcal{A})'$ such as

$$\chi(A)=(\Omega,\ B\pi_\omega(A)B\Omega),$$

where Ω is the G.N.S. cyclic vector induced by the state ω. The cyclicity of Ω implies that for any $\varepsilon>0$, there exists an element W in $\mathcal{A}$ such that $\|B^2\Omega-\pi_\omega(W)\Omega\|<\varepsilon$ holds. We hence have $|\chi(A)-\omega(AW)|<\varepsilon\|A\|$ for any $A\in\mathcal{A}$. (q. e. d.)

LEMMA. 2. *For the state $\phi=\phi^S\otimes\varphi^R$ introduced above, there exists an element K in $\mathcal{A}$ such that for any $\varepsilon>0$,*

$$|\phi(A)-\varphi(AK)|<\varepsilon\|A\|$$

for any $A\in\mathcal{A}$.

Proof. Let us consider two following subsets $\mathcal{V}^S$ and $\mathcal{D}^S$ of $\mathcal{S}^s$:

$$\mathcal{V}^S=\{\psi^S\in\mathcal{S}^S:\ \psi^S(A)=(\Psi^S,\ A\Psi^S)\text{ for any }A\in\mathcal{A}^S\text{ and }\Psi^S\in\mathcal{H}^S\}$$

and

$$\mathcal{D}^S=\{\psi^S\in\mathcal{S}^S:\ \psi^S\leqq\lambda\varphi^S\text{ for some }\lambda\in R^+\}.$$

As is known [13, 14], the set $\mathcal{V}^S$ is dense in $\mathcal{S}^S$ and the set $\mathcal{D}^S$ is dense in $\mathcal{V}^S$ because φ^S is a K.M.S. state. Hence for the state ϕ^S and any $\varepsilon>0$, there exists a state ω in $\mathcal{V}^S$ such that $|\phi^S(A)-\omega(A)|<(\varepsilon/3)\|A\|$ holds for any $A\in\mathcal{A}^S$. Moreover, for the above state ω, there exists a state χ in $\mathcal{D}^S$ such that $|\omega(A)-\chi(A)|<(\varepsilon/3)\|A\|$ for any $A\in\mathcal{A}^S$. As χ is dominated by φ^S, according to Lemma 1, there exists an element W in $\mathcal{A}^S$ such as $|\chi(A)-\varphi^S(AW)|<(\varepsilon/3)\|A\|$. We therefore obtain $|\phi(A)-\varphi(AK)|<\varepsilon\|A\|$ for any $A\in\mathcal{A}$, where K is taken as $K=W\otimes I^R$. (q. e. d.)

LEMMA 3. *For the state $\phi=\phi^S\otimes\varphi^R$, there exist a state ψ on $\mathcal{A}$ and an element R in $\mathcal{A}$ such that*

(i) *the state ψ satisfies the K.M.S. condition at β w.r.t. α_t, and*

(ii) *for any $\varepsilon>0$, $|\phi(A)-\psi(AR)|<\varepsilon\|A\|$ holds for any $A\in\mathcal{A}$.*

Proof. Let us introduce a vector as

$$\Psi=D^V\Phi/\|D^V\Phi\|,$$

where Φ is the cyclic vector associated with φ such that $\Phi=\Phi^S\otimes\Phi^R$ and $\varphi^S(A)=(\Phi^S, A\Phi^S)$ for any $A\in\mathcal{A}^S$, and D^V is given by

$$D^V=\sum_{n\geq 0}(-1)^n\int\limits_{0\leq t_1\leq\cdots\leq t_n\leq\beta/2} dt_1\cdots\int dt_n\tilde{\alpha}^0_{it_1}(\pi(V))\cdots\tilde{\alpha}^0_{it_n}(\pi(V)), \tag{2-1}$$

where $\tilde{\alpha}^0$ is the canonical extension of α^0 to the von Neumann algebra $\pi(\mathcal{A})''$. The above vector Ψ is always in the Hilbert space $\mathcal{H}$, although D^V is not in the C^*-algebra $\pi(\mathcal{A})$ except when V is a α^0-analytic element of $\mathcal{A}$. Define a state ψ by $\psi(A)=(\Psi, \pi(A)\Psi)$ for any $A\in\mathcal{A}$. This state ψ satisfies the K. M. S. condition at β w. r. t. α_t [10]. The state ψ and the time evolution automorphism α_t are constructed by φ and α^0_t through (2-1) and (1-6) respectively. Conversely, it is easily seen that φ and α^0_t can be constructed back from ψ and α_t with the interaction—V. Namely, putting $\Phi'=Q^V\Psi/\|Q^V\Psi\|$ with

$$Q^V=\sum_{n\geq 0}\int\limits_{0\leq t_1\leq\cdots\leq t_n\leq\beta/2} dt_1\cdots\int dt_n\tilde{\alpha}_{it_1}(\pi(V))\cdots\tilde{\alpha}_{it_n}(\pi(V)).$$

We can then readily show that $\Phi'=\Phi$. Moreover, by the simple but rather tedious computations using the boundary properties of the K. M. S. state, we obtain

$$\varphi(A)=(Q^V\Psi, \pi(A)Q^V\Psi)/\|Q^V\Psi\|^2=(\Psi, \pi(A)S^V_0\Psi),$$

where S^V_0 is given by $S^V/|(\Psi, S^V\Psi)|$ and

$$S^V=\sum_{n\geq 0}\int\limits_{0\leq t_1\leq\cdots\leq t_n\leq\beta} dt_1\cdots\int dt_n\tilde{\alpha}_{it_1}(\pi(V))\cdots\tilde{\alpha}_{it_n}(\pi(V)).$$

If the interaction V is a α^0-analytic (hence α-analytic) element of $\mathcal{A}$, the above S^V_0 is given by $\pi(\tilde{S}^V_0)$, where $\tilde{S}^V_0=\tilde{S}^V/|\psi(\tilde{S}^V)|$ and

$$\tilde{S}^V=\sum_{n\geq 0}\int\limits_{0\leq t_1\leq\cdots\leq t_n\leq\beta} dt_1\cdots\int dt_n\alpha_{it_1}(V)\cdots\alpha_{it_n}(V).$$

Since the set of all α-analytic element of $\mathcal{A}$ is dense in $\mathcal{A}$ in the norm topology, for any $V=V^*\in\mathcal{A}$ and any $\varepsilon>0$, there exists a α-analytic element $V_0=V_0{}^*\in\mathcal{A}$ such that $\|V-V_0\|<\varepsilon$. According to Theorem 3.1 of [10], we easily obtain

$$\|Q^V\Psi-Q^{V_0}\Psi\|<\frac{1}{2}\beta\|V-V_0\|\exp\Big(\frac{1}{2}\beta\|V-V_0\|\Big).$$

Hence for any $\varepsilon>0$, $\|Q^V\Psi/\|Q^V\Psi\|-Q^{V_0}\Psi/\|Q^{V_0}\Psi\|\|<\varepsilon$ holds. It is thus a easy exercise to show that for any $\varepsilon>0$, the inequality $|\varphi(A)-\psi(A\tilde{S}^{V_0}_0)|<\frac{1}{2}\varepsilon\|A\|$ is satisfied for any $A\in\mathcal{A}$. Now, by Lemma 2, there exists an element K in $\mathcal{A}$ such that $|\psi(A)-\varphi(AK)|<\frac{1}{2}\varepsilon\|A\|$ holds for any $A\in\mathcal{A}$. Taking $K\tilde{S}^{V_0}_0=R$, this R is an element of $\mathcal{A}$ and the inequality $|\psi(A)-\psi(AR)|<\varepsilon\|A\|$ holds for any $A\in\mathcal{A}$. (q. e. d.)

Let us find conditions under which every state $\phi=\phi^S\otimes\varphi^R$ ($\phi^S\in\mathcal{S}^S$) relaxes, under the time evolution α_t, to an equilibrium (K. M. S.) state at β w. r. t. α_t, as physically expected.

The spectrum of a Hamiltonian is one of the most important quantities of physics, and most of physicists are interested in the property of it; for example, how dense it is in R. In our case, the system considered is finite, so the spectrum of the Hamiltonian H^S is discrete, which forbids the approach to equilibrium. Therefore we needed some interaction with suitable reservoir. The Hamiltonian to be studied was the so-called total one $H=H^S+H^R+\pi(V)$. What we ask is the following: Which conditions do we have to impose on the total Hamiltonian H? In other words, which interaction V do we have to choose?

THEOREM 4. *If the rank of the projection E to the null space of H is one and the spectrum of H consists of $\{0\}$ and absolutely continuous one, then the time evolution automorphism α_t admits unique* K. M. S. *state ψ in the representation space $\mathcal{H}$ and the limit w^*-lim $\phi\circ\alpha_t$ is equal to ψ.*

Proof. In Lemma 3, we constructed the state ψ satisfying the K. M. S. condition w. r. t. α_t. For any A, $B\in\mathcal{A}$, let us consider $\psi(A\alpha_t(B))$, which is equal to $(\Psi, \pi(A)\exp(+itH)\pi(B)\Psi)$ because the K. M. S. state ψ is α_t-invariant. According to the spectral decomposition of H, we have

$$\psi(A\alpha_t(B))=(\pi(A)^*\Psi, \int\exp(+itr)de(r)\pi(B)\Psi).$$

When t tends to infinite, the above expression becomes

$$(\pi(A)^*\Psi, E\pi(B)\Psi)$$

because of the spectrum properties of H. Since the rank of E is one, $E\pi(B)\Psi=(\Psi, \pi(B)\Psi)\Psi$ for any $B\in\mathcal{A}$. We thus obtain

$$\lim_{|t|\to\infty}\psi(A\alpha_t(B))=\psi(A)\psi(B)$$

for any A, $B\in\mathcal{A}$. Namely the state ψ is clustering for α_t. This fact tells [13] that ψ is the unique K. M. S. state of $\mathcal{H}$. Let us now consider

$$|\phi(\alpha_t(A))-\psi(A)|,$$

which is less than

$$|\phi(\alpha_t(A))-\psi(\alpha_t(A)R)|+|\psi(\alpha_t(A)R)-\psi(A)|,$$

where R is an element in $\mathcal{A}$ obtained in Lemma 3. The first term of the above expression is again less than $\varepsilon\|A\|$ because of Lemma 3. We now estimate the second term:

$$I(t)=|\psi(\alpha_t(A)R)-\psi(A)|.$$

As shown that the state ψ is clustering for α_t and R is in $\mathcal{A}$,

$$\lim_{|t|\to\infty} I(t)=0$$

because of $\psi(R)=1$. We hence have

$$w^*\text{-}\lim_{|t|\to\infty} \phi\circ\alpha_t=\psi\,. \tag{q. e. d.}$$

We finally see what happens to the state ψ when the strength of the interaction V becomes very weak but the interaction still has the properties of Theorem 4.

THEOREM 5. *Under the conditions of Theorem* 4, *we have*

$$w^*\text{-}\lim_{\|V\|\to\infty}\ \lim_{|t|\to\infty} \phi\circ\alpha_t=\varphi^S \ \textit{on}\ \mathcal{A}^S.$$

Proof. From Theorem 4, we have only to show

$$w^*\text{-}\lim_{\|V\|\to 0} \psi=\varphi^S \ \text{on}\ \mathcal{A}^S\,.$$

As discussed in the proof of Lemma 3, the unique K. M. S. state ψ is given through $\psi(A)=(T^V\Phi,\ \pi(A)T^V\Phi)$ for any $A\in\mathcal{A}$, where T^V is given by

$T^V=D^V/\|D^V\Phi\|$ with D^V defined in the proof of Lemma 3.

Therefore the following inequality holds:

$$|\psi(A)-\varphi(A)|\leqq 2\|(I-T^V)\Phi\|\|A\|\,.$$

As mentioned in Lemma 3, for any $V=V^*\in\mathcal{A}$ and any $\varepsilon>0$, there exists a α^0-analytic element $V_0=V_0^*\in\mathcal{A}$ such that $\|T^V\Phi-T^{V_0}\Phi\|<\varepsilon$. We hence have

$$|\psi(A)-\varphi(A)|\leqq 2\|(I-T^{V_0})\Phi\|\|A\|\,.$$

The above inequality together with the facts that $T^{V_0=0}=I$ implies that $w^*\text{-}\lim_{\|V\|\to 0}\psi=\varphi$ on $\mathcal{A}$. As the restriction of the state φ to $\mathcal{A}^S$ is φ^S, we have the conclusion. (q. e. d.)

This theorem shows that if we can choose the interaction so that its strength is sufficiently weak but the total Hamiltonian $H=H^S+H^R+\pi(V)$ still satisfies the condition of Theorem 4, then the limiting state of ψ under $\|V\|\to 0$ is enough close to the equilibrium state φ, that is, any state ϕ^S on $\mathcal{A}^S$ approaches to the equilibrium state φ^S in the above sense.

The theorem 4 will be somewhat related to the derivation of equilibrium state [15, 16], about which we will discuss elsewhere. The conditions of Theorems 4 and 5 might be realized in some physical models.

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