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Theory of Quantum Fluctuations and the Onsager Relations

D. Goderis,[1,2] **A. Verbeure,**[1] **and P. Vets**[1,2]

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A microscopic model is constructed within the theory of normal fluctuations for quantum systems, yielding an irreversible dynamics satisfying the Onsager relations. The property of return to equilibrium and the principle of minimal entropy production are proved.

KEY WORDS: Quantum central limit theorem; macroscopic fluctuations; Onsager relation; minimal entropy production.

1. INTRODUCTION

In this paper we derive from the microscopic theory a number of assumptions in the phenomenological macroscopic Onsager theory. This theory should follow straightforwardly from the microscopic laws of motion and from the principles of statistical mechanics.

In the classical Onsager theory (see, e.g., ref. 1), one is interested in a finite number of macroscopic variables or observables $A_1,..., A_n$, namely the "coarse-grained" ones. One considers a phase space Γ; any element $\alpha = (\alpha_1,..., \alpha_n)$ of Γ represents a state of the system by the association $\alpha_i = \langle A_i \rangle$, i.e., the α_i are the expectation values of the observables A_i. The equilibrium state is assumed to correspond to the value $\alpha = 0$, and postulated to be the state of minimal entropy. One more basic assumption is that the α_i are Gaussian random variables with distribution

$$f(\alpha) = f(0)\, e^{-(\alpha, S\alpha)/2}, \qquad S \geqslant 0$$

[1] Instituut voor Theoretische Fysica, Universiteit Leuven, B-3030 Leuven, Belgium.
[2] Onderzoeker IIKW, Belgium.

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and that the α_i describe a regime not far from equilibrium. The Boltzmann entropy postulate yields the identification of the entropy difference ΔS with

$$\frac{\Delta S}{k} = \frac{S(\alpha) - S(0)}{k} = -\frac{1}{2}(\alpha, S\alpha)$$

where $S(\alpha)$ is the entropy of the state α and k the Boltzmann constant. The above formula is looked upon as the harmonic approximation or the linear response expression of the entropy around the equilibrium state.

One of the basic results of the Onsager theory are the Onsager relations, which are the macroscopic expression of the microscopic reversibility of the equations of motion. It is our aim to derive these results in a mathematically rigorous way. It is well known that a natural scheme for all this is the theory of fluctuations, the latter being the result of a central limit theorem.

Recently, we developed the mathematical theory of fluctuations for quantum mechanical systems. We will use it to derive the basic facts of the theory of Onsager for quantum systems. In refs. 2 and 3 central limit theorems are derived for sets of noncommuting observables as well as for product states and for mixing states. A complete mathematical description of the central limits is obtained. The set of macroscopic fluctuations forms again a noncommutative algebra, namely a representation of the canonical commutation relations induced by a generalized free or quasifree state. This is the natural generalization of the classical random variable with Gaussian distribution in the commutative case. It is also pointed out how the natural conservative time evolution of the system induces a nontrivial time evolution on the macroscopic fluctuations. This clarifies and generalizes the computations of these time evolutions performed for the examples of mean field models (e.g., refs. 4 and 5). It enables us also to interpret the quasifree limit state as the equilibrium state of the macrosystem of fluctuations. Our program here is the study of nonequilibrium phenomena within the above scheme of the mathematical theory of fluctuations.

The physical situation which we consider here is the usual one, namely the evolution of the fluctuations of the system driven by heat reservoirs. Numerous models for this mechanism have been studied (see, e.g., ref. 6 for a recent model). We work with a microscopic model obtained as the result of a weak coupling limit satisfying a quantum generalization of a classical Markov process. The natural time evolution of the microscopic model is the Heisenberg evolution α_t described by a Hamiltonian H. We limit our discussion here to systems with continuous spectrum. This is characterized by the condition of L^1-asymptotically Abelianness

$$\int_{-\infty}^{\infty} ds \, \|[\alpha_s(X), Y]\| < \infty$$

for a large set of observables X and Y of the system. If the spectrum of the Hamiltonian is discrete, the main results of the paper remain true; the proofs are similar but are not given here. Furthermore, we suppose that the system is given in an equilibrium state ω at inverse temperature β, which we normalize to $\beta = 1$, showing normal fluctuations for enough observables. The latter condition is at least always satisfied if the temperature is high enough.

Then we consider an irreversible dynamics by coupling the microscopic model to a heat reservoir R. The interaction Hamiltonian system–reservoir H_{SR} is of the type

$$H_{SR}^V = \lambda \int_{x \in V} dx \, \frac{[X(x) - \omega(X)] \, Z}{\sqrt{V}}$$

where $X^* = X$ is a system observable and $Z^* = Z$ is a bath observable. For fixed volume V, applying the weak coupling limit yields an irreversible Markovian evolution $\exp(tL_V)$. A precise definition of L_V is given in formula (3.1) below. It is well known that this evolution is microreversible or in other words satisfies the condition of detailed balance. It expresses the fact that the heat reservoirs are at thermal equilibrium. It is clear that the coupling of the system with the reservoirs is of a very special type because of the presence of the volume integral divided by the square root of the volume. The effect in the generator L_V of the Markovian evolution is such that the coupling becomes of the mean field type.

Our main technical contribution consists in the study of the thermodynamical limit $L_V \to L$ for the volume V tending to infinity. We consider this limit as a central limit and derive the very specific form of the limit L. We identify L as a map of the algebra of macroscopic fluctuations in itself. We prove that L is exponentiable to a semigroup of quasifree maps on the fluctuations. This is a macroscopic dynamical semigroup for which we show the symmetry relations of the Onsager theory. The program of irreversible thermodynamics for quantum systems has been studied by Spohn and Lebowitz.[9] Their coupling, however, was a local one, such that their results hold only in the linear regime (see also ref. 10). In fact, we show here that the linear regime results become exact if one takes mean field type couplings. Differently formulated, the Onsager theory becomes exact if the system shows normal fluctuations. Moreover, we clarify the notion of entropy production and prove the phenomenon of approach to equilibrium and the principle of minimal entropy production for infinite systems.

2. THE MODEL

Our basic starting point is a quantum mechanical system given by the triplet $(\mathscr{A}, \rho, \alpha_t)$, where $\mathscr{A}$ is a unital C^*-algebra of observables, $(\alpha_t)_t$ is a strongly continuous one-parameter group of *-automorphisms, and ρ is an equilibrium or KMS state of $(\mathscr{A}, \alpha_t)$ at inverse temperature $\beta = 1$, i.e., for all x, y in a norm dense *-subalgebra $(\mathscr{A}_\alpha)$ of $\mathscr{A}$ consisting of the α_t-analytic elements, one has[11]

$$\rho(x\alpha_i y) = \rho(yx)$$

It is well known that the state ρ is α_t or time invariant.

We define the algebra of normal fluctuations of the physical system $(\mathscr{A}, \rho)$ as the CCR-C^*-algebra $W(H, \sigma_\rho)$,[2] where we take $H = \mathscr{A}_{\text{sa}}$ the real space of self-adjoint elements of the algebra $\mathscr{A}$ and where σ_ρ is the symplectic form on $\mathscr{A}_{\text{sa}}$:

$$\sigma_\rho(x, y) = -i\rho([x, y]); \qquad x, y \in \mathscr{A}_{\text{sa}} \tag{2.1}$$

The algebra $W(\mathscr{A}_{\text{sa}}, \sigma_\rho)$ is the C^*-algebra generated by the Weyl operators $W(x)$, $x \in \mathscr{A}_{\text{sa}}$, satisfying the product rule

$$W(x)\, W(y) = W(x + y)\, e^{-i\sigma_\rho(x, y)/2} \tag{2.2}$$

The fact that this algebra of canonical commutation relations (CCR) is the algebra of normal fluctuations of the system becomes clear from the following central limit theorem, which we formulate for independent random operators. The noncommutative central limit theorem for weakly dependent random operators or for mixing systems can be found in ref. 3.

A natural way of introducing a quantum mechanical notion of independence is via the tensor product construction of the algebra of observables and the product property of the state.

Consider the C^*-algebra $\mathscr{B}$, generated by the sequence of algebras

$$\tilde{\mathscr{A}}_n = \bigotimes_{i=1}^{n} \mathscr{A}_i, \qquad n = 1, 2, 3,\ldots$$

where the $\mathscr{A}_i$ are copies of $\mathscr{A}$. For each $x \in \mathscr{A}$, denote by x_i the imbedding of x in $\mathscr{B}$,

$$x_i = 1 \otimes \cdots \otimes x \otimes 1 \otimes \cdots$$

where x is at the ith place. Denote

$$\tilde{x}^n = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} [x_i - \rho(x)] \in \mathscr{B}$$

the local (n is finite) fluctuation of x.

Consider also the product state ω_ρ of $\mathscr{B}$ determined by the given state ρ of $\mathscr{A}$ and defined by

$$\omega_\rho\left(\bigotimes_{j=1}^{n} a_j\right)=\prod_{j=1}^{n} \rho(a_j); \qquad a_j \in \mathscr{A}$$

In this way we define a lattice system $(\mathscr{B}, \omega_\rho)$. Now we are able to give the following noncommutative central limit theorem. Its proof in the W^* formulation can be found in ref. 2, Theorem 3.1. For this case the proof can be readily transcribed.

Theorem 2.1. For each $x \in \mathscr{A}_{\text{sa}}$, the limit

$$\lim_{n \to \infty} \omega_\rho(\exp i\tilde{x}^n)$$

exists and defines a quasifree state ω_s (see ref. 12) of the CCR-C^*-algebra of fluctuations $W(\mathscr{A}_{\text{sa}}, \sigma_\rho)$ such that

$$\lim_{n \to \infty} \omega_\rho(\exp i\tilde{x}^n)=\omega_s(W(x))=\exp\left[-\frac{1}{2}s(x, x)\right] \tag{2.3}$$

where s is the real, symmetric, positive bilinear form on $\mathscr{A}_{\text{sa}}$ given by

$$s(x, y)=\text{Re}\,\rho([x-\rho(x)][y-\rho(y)]); \qquad x, y \in \mathscr{A}_{\text{sa}} \quad \blacksquare$$

As the quasifree state ω_s is a regular state, the Weyl operators $W(x)$ are represented by exponentials of the Bose field operator $B_\rho(x)$:

$$W(x)=\exp iB_\rho(x), \qquad x \in \mathscr{A}_{\text{sa}} \tag{2.4}$$

satisfying the commutation relations $[B_\rho(x), B_\rho(y)]=i\sigma_\rho(x, y)$. In view of the relation (2.3), one can make the identification

$$B_\rho(x)=\text{“}\lim_{n \to \infty}\text{”}\, \tilde{x}^n$$

suggesting the interpretation that the unbounded operators $B_\rho(x)$ are nothing but the (macroscopic) fluctuations of the observables $x \in \mathscr{A}_{\text{sa}}$.

In the commutative case (for classical systems) the algebra of fluctuations is again commutative. The quasifree state ω_s reduces in that case to a Gaussian measure.

The natural time evolution α_t defined on the system $(\mathscr{A}, \rho)$ induces a conservative time evolution on the algebra of fluctuations. In particular, we have the following result.

Theorem 2.2 (ref. 2, Theorem 3.3). For $t \in \mathbb{R}$, the maps $\tilde{\alpha}_t$ defined by the formula

$$\tilde{\alpha}_t W(x) = W(\alpha_t x), \qquad x \in \mathscr{A}_{\text{sa}}$$

define a one-parameter group of quasifree *-automorphisms of the algebra of fluctuations $W(\mathscr{A}_{\text{sa}}, \sigma_\rho)$. The state ω_s is an $\tilde{\alpha}_t$-KMS state at $\beta = 1$ on the von Neumann algebra $W(\mathscr{A}_{\text{sa}}, \sigma_\rho)''$, generated by the representation of the C^*-algebra induced by the state ω_s.

So far for the equilibrium statistical mechanics. In this paper we are interested in irreversible thermodynamics. We introduce an irreversible evolution, a quantum generalization of a classical Markov process, which satisfies the detailed belance condition. Here we define the evolution on the original system $(\mathscr{A}, \rho)$ and show in the next sections that it induces a bona fide irreversible evolution on the fluctuation algebra. Suppose that the system $(\mathscr{A}, \alpha_t)$ is L^1-asymptotically Abelian, i.e., there exists a norm dense *-subalgebra $\mathscr{A}_0$ of $\mathscr{A}$ such that

$$\int_{-\infty}^{\infty} ds \, \| [\alpha_s x, y] \| < \infty$$

for all $x, y \in \mathscr{A}_0$.

Assume also that $\mathscr{A}_0 \subseteq \mathscr{A}_\alpha$, the analytical elements of $\mathscr{A}$ for α_t.

Consider now the maps

$$L_x^f(\cdot) = \int_{-\infty}^{\infty} dt \, ds \, f(t) \{ \alpha_s(x) [\cdot, \alpha_{s+t} x] + [\alpha_s x, \cdot] \, \alpha_{s+t} x \} \tag{2.5}$$

for all $x = x^* \in \mathscr{A}_0$ and f a complex function satisfying the following:

(i) f is analytical in the strip $\{z \in \mathbb{C} \mid 0 < \text{Im}\, z < 1\}$, and continuous and bounded on its closure.

(ii) f is analytic in t$\mathbb{R}$, dt).

(iii) $f \in L^1(\mathbb{R}, dt)$.

(iv) $t \to f(t)$ is of positive type.

Remark that the Fourier transform $\hat{f}$ of f exists and satisfies

(iii)′ $\hat{f}(-\lambda) = \hat{f}(\lambda) \, e^{-\lambda}$.

(iv)′ $\hat{f}(\lambda) > 0$.

The integrals in (2.5) are in the norm sense. It is well known[8] that the maps L_x^f are densely defined, dissipative maps of $(\mathscr{A}, \rho)$ satisfying the condition of detailed balance with respect to ρ, i.e., for all y_i $(i=1, 2)$ in the domain of L_x^f we have

$$L_x^f(y_1 y_2) - L_x^f(y_1)\, y_2 - y_1 L_x^f(y_2) \geqslant 0 \qquad \text{(dissipativity)}$$

$$\rho(L_x^f(y_1)\, y_2) = \rho(y_1 L_x^f(y_2)) \tag{2.6}$$

(detailed balance or microreversibility)

These maps can be derived from a microscopic interaction between the system and a heat reservoir in the weak coupling limit.[13] Formally they are of the type of generators of semigroups of completely positive maps.[14]

We will develop the theory for L^1-asymptotically Abelian systems $(\mathscr{A}, \alpha_t, \rho)$. Technically, the finite-dimensional systems [i.e., $\mathscr{A} = \mathscr{B}(\mathscr{H})$ with $\dim \mathscr{H} < \infty$; see ref. 9] are excluded. However, this case, being even easier, can be done along the same lines by replacing one of the time integrals in formula (5) by a mean.

We complete this section by deriving some spectral properties for the system $(\mathscr{A}, \alpha_t, \rho)$ introduced above.

Lemma 2.3. Let μ be a positive, regular, Borel measure on $\mathbb{R}$ with compact support; then its Fourier transform

$$\hat{\mu}(t) = \int e^{-it\lambda}\, d\mu(\lambda)$$

exists. If $\hat{\mu} \in L^1(\mathbb{R}, dt)$, then μ is absolutely continuous w.r.t. the Lebesque measure and

$$\frac{d\mu(\lambda)}{d\lambda} = \int dt\, e^{it\lambda} \hat{\mu}(t)$$

Proof. Denote $R(\lambda) = \int dt\, e^{it\lambda} \hat{\mu}(t)$. As $\hat{\mu}$ is the Fourier transform of a finite positive measure, it is of positive type and $\overline{R(\lambda)} = R(\lambda)$. Hence, for all test functions φ and using $\hat{\mu} \in L^1(\mathbb{R}, dt)$,

$$\int d\lambda\, R(\lambda)\, \varphi(\lambda) = \int dt\, \hat{\varphi}(-t)\, \hat{\mu}(t)$$

$$= \int dt\, \hat{\varphi}(-t) \int e^{-it\lambda}\, d\mu(\lambda) = \int \varphi(\lambda)\, d\mu(\lambda)$$

Therefore $R(\lambda)\, d\lambda = d\mu(\lambda)$ in the sense of distributions. As μ is regular and of bounded support, the test-function space is dense in $L^1(\mathbb{R}, d\mu)$ (Ref. 15, Theorem IV.13), and

$$\int f(\lambda)\, d\mu(\lambda) = \int f(\lambda)\, R(\lambda)\, d\lambda$$

for all $f \in L^1(\mathbb{R}, d\mu)$. ∎

Consider now the GNS representation of $\mathscr{A}$ induced by the state ρ; denote by $\mathscr{M}_\rho = \mathscr{A}_0''$ the von Neumann algebra generated by $\mathscr{A}_0$ or by $\mathscr{A}$. If Ω_ρ is the cyclic vector of the representation, then the representation space $\mathscr{H}_\rho$ is generated by the set $\mathscr{M}_\rho \Omega_\rho$. Because of the KMS property of the state ρ, the cyclic vector Ω_ρ is also separating for $\mathscr{M}_\rho$.

Denote by H_ρ the GNS Hamiltonian acting on $\mathscr{H}_\rho$:

$$\alpha_t(x)\, \Omega_\rho = e^{itH_\rho} x \Omega_\rho; \qquad x \in \mathscr{A}$$

and by E_ρ the projection operator on the time-invariant subspace of $\mathscr{H}_\rho$.

Let

$$H_\rho = \int \lambda\, dE_{-\lambda}$$

be the spectral representation of H_ρ. For $\psi \in \mathscr{H}_\rho$, denote the associated spectral measure by

$$d\mu_\psi(\lambda) = (\psi, dE_{-\lambda} \psi)$$

Its spectral support is then

$$\Delta_\psi = \{\lambda \in \mathbb{R} \mid \mu_\psi([\lambda - \varepsilon, \lambda + \varepsilon]) > 0 \text{ for all } \varepsilon > 0\}$$

Clearly, Δ_ψ is the support of the Fourier transform of $t \to (\psi, e^{itH_\rho}\psi)$.

If $\psi = z\Omega_\rho$, $z \in \mathscr{A}$, we write for simplicity $d\mu_z$, Δ_z for $d\mu_{\psi = z\Omega_\rho}$, $\Delta_{\psi = z\Omega_\rho}$ and call Δ_z the spectral support of z. For $f \in L^1(\mathbb{R}, dt)$, denote

$$x(f) = \int dt\, f(t)\, \alpha_t x; \qquad x \in \mathscr{A}$$

Because

$$\int dt\, \|[\alpha_t x(f), y]\| \leqslant \|f\|_1 \int dt\, \|[\alpha_t x, y]\|$$

we may always assume that $x(f) \in \mathscr{A}_0$ for $x \in \mathscr{A}_0$. Finally, remark also that

$$x(f)\, \Omega_\rho = \int \hat{f}(\lambda)\, dE_\lambda\, x\Omega_\rho = \hat{f}(-H_\rho)\, x\Omega_\rho$$

Proposition 2.4. If $x \in \mathscr{A}_0$ such that $0 \notin \Delta_x$ and Δ_x is bounded, then the spectral measure μ_x is absolutely continuous w.r.t. the Lebesgue measure and

$$\frac{d\mu_x(\lambda)}{d\lambda} = \frac{1}{1-e^{-\lambda}} \int dt\, e^{-it\lambda} \rho([x^*, \alpha_t x])$$

Proof. Take $f \in L^1(\mathbb{R}, dt)$ satisfying the conditions of (2.5). Let $g(t) = f(t) - f(-t)$; then $g \in L^1(\mathbb{R}, dt)$ and

$$\hat{g}(\lambda) = -\hat{g}(-\lambda) = \hat{f}(\lambda)(1-e^{-\lambda})$$

Denote the finite positive measure [(2.5), property (iv′)]

$$d\nu_f(\lambda) = \hat{f}(\lambda)(1-e^{-\lambda})^2\, d\mu_x(\lambda)$$

Using the KMS property of ρ (ref. 11, Theorem 5.3.14)

$$\frac{d\mu_{x^*}(-\lambda)}{d\mu_x(\lambda)} = e^{-\lambda}$$

and one gets, using (2.5), property (iii′),

$$\begin{aligned}
&\int e^{-it\lambda}\, d\nu_f(\lambda) \\
&\quad = \int e^{-it\lambda} \hat{g}(\lambda)[(x\Omega_\rho, dE_{-\lambda} x\Omega_\rho) - (x^*\Omega_\rho, dE_\lambda x^*\Omega_\rho)] \\
&\quad = -\rho([x^*, \alpha_{-t} x(g)])
\end{aligned}$$

As $x \in \mathscr{A}_0$, the Fourier transform of ν_f is an L^1-function. By Lemma 2.3,

$$\frac{d\nu_f(\lambda)}{d\lambda} = -\int dt\, e^{it\lambda} \rho([x^*, \alpha_{-t} x(g)])$$

Using the L^1-property of g, one computes

$$\begin{aligned}
\frac{d\nu_f(\lambda)}{d\lambda} &= -\int dt\, e^{it\lambda} \left\{ \int ds\, g(s)\, \rho([x^*, \alpha_{-t+s} x]) \right\} \\
&= \hat{f}(\lambda)(1-e^{-\lambda}) \int dt\, e^{-it\lambda} \rho(x^*, \alpha_t x)
\end{aligned}$$

The proposition follows from the fact that $0 \notin \Delta_x$, Δ_x being bounded, and (2.5), property (iv′). ∎

In the following, we wil also assume that ρ is a factor state. Hence ρ is an extremal KMS state. Together with the L^1-asymptotic Abelianness of the system, this implies that the state ρ is strongly clustering (ref. 11, Theorem 4.3.24), and that E_ρ is the rank-one projection on the cyclic vector Ω_ρ (ref. 11, Theorems 4.3.20, 4.3.23). For completeness the spectral properties of such systems can be summarized as follows:

Proposition 2.5. Let $(\mathscr{A}, \alpha_t)$ be an L^1-asymptotic Abelian system and ρ an extremal KMS state; then the absolutely continuous spectrum of H_ρ is $\mathbb{R}$, the point spectrum of H_ρ is $\{0\}$, and the singular continuous spectrum of H_ρ is empty.

Proof. Clearly

$$\mathscr{H}_\rho = E_\rho \mathscr{H}_\rho \oplus (1 - E_\rho)\, \mathscr{H}_\rho$$

From spectral theory we know that $(1 - E_\rho)\, \mathscr{H}_\rho$ is the closure of the set

$$\{x\Omega_\rho \mid x \in \mathscr{A}_0, 0 \notin \Delta_x, \Delta_x \text{ bounded}\}$$

By Proposition 2.4, $(1 - E_\rho)\, \mathscr{H}_\rho$ is the absolutely continuous spectral subspace; $E_\rho \mathscr{H}_\rho$ is the point spectral subspace and hence there is no singular continuous spectrum. Finally, that the spectrum is $\mathbb{R}$ follows from ref. 11, Theorem 4.3.28. ∎

3. CENTRAL LIMIT THEOREM

First we extend the map L_x^f of (2.5) on $(\mathscr{A}, \rho)$ to the system $(\mathscr{B}, \omega_\rho)$. We substitute in (2.5) the observable $x \in \mathscr{A}_{0,\mathrm{sa}}$ by its local fluctuation:

$$\tilde{x}^n = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} [x_i - \rho(x)] \in \mathscr{B}$$

and obtain as a densely defined map of $\mathscr{B}$

$$L_{\tilde{x}^n}^f = \int_{-\infty}^{\infty} ds \{\alpha_s(\tilde{x}^n)[\,\cdot\,, \alpha_s(\tilde{x}(f)^n)] + [\alpha_s(\tilde{x}^n), \cdot\,]\, \alpha_s(\tilde{x}(f)^n)\} \tag{3.1}$$

Remark that the set

$$\bigcup_n \left(\bigotimes_{i=1}^{n} \mathscr{A}_0 \right)$$

is in the domain of $L_{\tilde{x}^n}^f$. From now on, we work with a fixed observable $x \in \mathscr{A}_{0,\mathrm{sa}}$ and a fixed function f.

Here we prove by a central limit theorem that the limit $n \to \infty$ of (3.1) yields a map on the algebra of fluctuations $W(\mathscr{A}_{\text{sa}}, \sigma_\rho)$. In Section 4, we prove that this map is exponentiable on this algebra and yields a semigroup of unitary preserving completely positive maps. Such semigroups are called dynamical semigroups.

Lemma 3.1. If $x, y \in \mathscr{A}_{0,\text{sa}}$, then for all $n \in \mathbb{N}$, $\exp i\tilde{y}^n$ belongs to the domain of the map $L^f_{\tilde{x}^n}$ of (3.1).

Proof. Clearly $\tilde{y}^n$ belongs to the domain because of the bound

$$\|L^f_{\tilde{x}^n}(\tilde{y}^n)\| \leqslant 2\sqrt{n} \int dt\, |f(t)|\ \ \|x\| \int ds\, \|[y, \alpha_s x]\|$$

Using the inequality

$$\|[e^{iz_1}, z_2]\| \leqslant \|[z_1, z_2]\|$$

for all z_1, z_2 elements of a C^*-algebra such that $z_1^* = z_1$, one gets the same bound as above for

$$\|L^f_{\tilde{x}^n}(\exp i\tilde{y}^n)\|$$

proving that $\exp i\tilde{y}^n$ also belongs to the domain of $L^f_{\tilde{x}^n}$. ∎

Now we have the following central limit theorem.

Theorem 3.2. For all $z_1, z_2 \in \mathscr{A}_{\text{sa}}$ and $x, y \in \mathscr{A}_{0,\text{sa}}$,

$$\lim_{n \to \infty} \omega_\rho((\exp i\tilde{z}_1^n)\, L^f_{\tilde{x}^n}(\exp i\tilde{y}^n) \exp i\tilde{z}_2^n)$$

$$= \omega_s(W(z_1)\, L_\rho(W(y))\, W(z_2)) \tag{3.2}$$

where L_ρ is understood as a map on the GNS representation of the fluctuations induced by ω_s:

$$L_\rho(W(y)) = (iB_\rho(\Gamma_\rho y) + \chi_\rho(y))\, W(y)$$

Γ_ρ is a linear map of $\mathscr{A}$:

$$\Gamma_\rho(y) = \int ds\{\alpha_s x \rho([y, \alpha_s x(f)]) + \rho([\alpha_s x, y])\, \alpha_s x(f)\} \tag{3.3}$$

χ_ρ is a functional on $\mathscr{A}$:

$$\chi_\rho(y) = \int ds\, \rho([y, \alpha_s x])\, \rho([y, \alpha_s x(f)]) \leqslant 0$$

and finally $B_\rho(\cdot)$ is defined in (2.4).

Proof. By Lemma 3.1, the expressions in (3.2) are well defined. For notational convenience, we redefine all operators $x, y, \ldots$ such that $\rho(x) = \rho(y) = \cdots = 0$. Remark that using the product property of ω_ρ, we have

$$\begin{aligned}
&\lim_{n \to \infty} \omega_\rho(\exp i\tilde{x}^n \exp i\tilde{y}^n \cdots) \\
&= \lim_{n \to \infty} \rho\left(\exp i\frac{x}{\sqrt{n}} \exp i\frac{y}{\sqrt{n}} \cdots\right)^n \\
&= \lim_{n \to \infty} \left[1 - \frac{1}{n}\rho\left(xy + \frac{x^2}{2} + \frac{y^2}{2} + \cdots\right) + O\left(\frac{1}{n^{3/2}}\right)\right]^n \\
&= \exp -\frac{1}{2}\left[\rho(x^2) + \rho(y^2) + 2\rho(xy) + \cdots\right] \\
&= \exp\left\{-\frac{1}{2}s(x + y + \cdots, x + y + \cdots) - \frac{i}{2}\sigma_\rho(x, y) - \cdots\right\} \\
&= \omega_s(W(x)\, W(y) \cdots) \qquad (*)
\end{aligned}$$

For the last step we used the product rule for Weyl operators (2.2) and Theorem 2.1. In fact, the property (*) is a straightforward extension of that theorem. Analogously, one gets

$$\lim_{n \to \infty} \omega_\rho\left((\exp i\tilde{x}^n)\left(\frac{1}{n}\sum_{j=1}^{n} y_j\right)\exp i\tilde{z}^n\right) = \omega_s(W(x)\, W(z))\, \rho(y) \qquad (**)$$

$$\lim_{n \to \infty} \omega_\rho\left((\exp i\tilde{x}^n)\, \tilde{y}^n \exp i\tilde{z}^n\right) = \omega_s(W(x)\, B_\rho(y)\, W(z)) \qquad (***)$$

for all x, y, z in $\mathscr{A}_{\text{sa}}$. Consider now the map $L^f_{\tilde{x}^n}$. Using the formula

$$[e^{iy}, x] = i\int_0^1 du\, e^{iuy}[y, x]\, e^{i(1-u)y}$$

for x and y, elements of a C^*-algebra, one gets

$$\begin{aligned}
&\lim_{n \to \infty} \omega_\rho((\exp i\tilde{z}_1^n)\, L^f_{\tilde{x}^n}(\exp i\tilde{y}^n) \exp i\tilde{z}_2^n) \\
&\quad = \lim_{n \to \infty} \int dt\, ds\, f(t)\, i\int_0^1 du\, \omega_\rho((\exp i\tilde{z}_1^n)\, \alpha_s\tilde{x}^n(\exp iu\tilde{y}^n)) \\
&\qquad + \frac{1}{n}\sum_{j=1}^{n} [y_j, \alpha_{s+t}x_j] \exp[i(1-u)\, \tilde{y}^n] \exp(i\tilde{z}_2^n) + \cdots
\end{aligned}$$

Using (*), (**), (***), the Lebesgue dominated convergence theorem, and the commutation relation (2.2) in the form

$$[W(y), B_\rho(x)] = \sigma(x, y)\, W(y)$$

one gets as limit

$$\omega_s(W(z_1)\, L_\rho(W(y))\, W(z_2)) \quad \blacksquare$$

Remark that the limit map L_ρ depends on the chosen $x \in \mathscr{A}_{0,\mathrm{sa}}$ and the chosen function f [see (2.5)]. For notational convenience, we omit the indices x and f. However, the ρ-state dependence of this limit is one of the essential outcomes of the above theorem. This is indicated by the index ρ.

The limit map L_ρ has the same structure as the original map L_x^f, in the sense that a formal computation yields

$$\begin{aligned} L_\rho(W(y)) &= L_{B_\rho(x)}(W(y)) \\ &= \int dt\, ds\, f(t)\{\tilde{\alpha}_s B_\rho(x)[W(y), \tilde{\alpha}_{s+t} B_\rho(x)] \\ &\quad + [\tilde{\alpha}_s B_\rho(x), W(y)]\, \tilde{\alpha}_{s+t} B_\rho(x)\}; \qquad y \in \mathscr{A}_{0,\mathrm{sa}} \end{aligned}$$

where $\tilde{\alpha}$ is the quasi-free time evolution of the fluctuations (Theorem 2.2). The map L_ρ has, however, the important property that it maps monomials in the field operators, say of order n, into linear combinations of monomials of field operators of order less than or equal to n. This kind of map is called a quasifree map. As an illustration, we give the map L_ρ explicitly on the monomials of order one and two:

$$\begin{aligned} L_\rho(B_\rho(y)) &= B_\rho(\Gamma_\rho y) \\ L_\rho(B_\rho(y)^2) &= B_\rho(\Gamma_\rho y)\, B_\rho(y) + B_\rho(y)\, B_\rho(\Gamma_\rho y) - 2\chi_\rho(y) \end{aligned}$$

In fact, it turns out that these two formulas are sufficient to characterize completely the L_ρ on the whole CCR-algebra of fluctuations.

4. MACROSCOPIC DYNAMICS SATISFYING THE ONSAGER RELATIONS

First we prove that the map L_ρ of Theorem 3.2 is the generator of a dynamical semigroup on the von Neumann algebra $W(\mathscr{A}_{\mathrm{sa}}, \sigma_\rho)''$ generated by the fluctuation CCR-algebra and induced by the quasifree state ω_s (see Theorem 2.1).

In general a dynamical semigroup[14,16,17] on a von Neumann algebra $\mathscr{M}$ is a one-parameter semigroup $\{\gamma_t \mid t \in \mathbb{R}^+\}$ such that:

(i) γ_t is a completely positive map of $\mathscr{M}$ for all $t \geqslant 0$.

(ii) $\gamma_t(\mathbb{1}) = \mathbb{1}$.

(iii) γ_0 is the identity map.

(iv) γ_t is a normal map for all $t \geqslant 0$.

(v) $t \to \gamma_t(X)$ is ultraweakly continuous for all $X \in \mathscr{M}$.

If one has given such a dynamical semigroup γ_t, then it defines a generator L. The domain of L is the set of all $X \in \mathscr{M}$ such that

$$\text{u.w.} \lim_{t \to 0^+} \frac{\gamma_t(X) - X}{t}$$

exists. The limit itself defines the generator L.

We begin with the study of the map Γ_ρ of $\mathscr{A}$ with domain $\mathscr{A}_0$ and given by

$$\Gamma_\rho(y) = \int ds \{\alpha_s x \rho([y, \alpha_s x(f)]) + \rho([\alpha_s x, y])\, \alpha_s x(f)\}, \qquad y \in \mathscr{A} \tag{4.1}$$

Lemma 4.1. The map Γ_ρ satisfies:

(i) $\Gamma_\rho(\mathbb{1}) = 0$.

(ii) Γ_ρ is Hermitian: i.e., $\Gamma_\rho(y)^* = \Gamma_\rho(y^*)$; $y \in \mathscr{A}_0$.

(iii) Γ_ρ is symmetric with respect to ρ; i.e., for all $y, z \in \mathscr{A}_0$

$$\rho(y \Gamma_\rho z) = \rho(\Gamma_\rho(y)\, z)$$

(iv) $\rho \circ \Gamma_\rho = 0$.

(v) Γ_ρ is negative definite with respect to ρ, i.e., for all $y \in \mathscr{A}_0$

$$\rho(y^* \Gamma_\rho\, y) \leqslant 0$$

Proof. Part (i) is trivial

(ii) Compute

$$\Gamma_\rho(y)^* = \int dt\, ds\, \bar{f}(t) \{\alpha_s x \rho([\alpha_{s+t} x, y^*]) + \alpha_{s+t} \rho([y^*, \alpha_s x])\}$$

Performing the coordinate transformations $s + t \to s$ and $t \to -t$, one gets

$$\begin{aligned} \Gamma_\rho(y)^* &= \int dt\, ds\, \bar{f}(-t) \{\alpha_s x \rho([\alpha_{s+t} x, y^*]) \\ &\quad + \alpha_{s+t} \rho([y^*, \alpha_{s+t} x])\} \\ &= \Gamma_\rho(y^*) \end{aligned}$$

The last equality follows from $\bar{f}(-t)=f(t)$ [see (2.5)]. The proof of (iii) is analogous to the proof of Theorem 2.2 of ref. 8; (iv) follows from (i) and (iii). To prove (v), remark that

$$\begin{aligned}\rho(y^*\Gamma_\rho y) &= \int dt\, ds\, f(t)\{\rho([y, \alpha_{s+t}x])\,\rho(y^*\alpha_s x) \\ &\quad + \rho([\alpha_s x, y])\,\rho(y^*\alpha_{s+t}x)\} \\ &= \int dt\, ds\, f(t-s)\{\rho([y, \alpha_t x])\,\rho(y^*\alpha_s x) \\ &\quad + \rho([\alpha_s x, y])\,\rho(y^*\alpha_t x)\}\end{aligned}$$

For fixed s, consider the function

$$t \to F(t, s) = f(t-s)\,\rho([\alpha_s x, y])\,\rho(y^*\alpha_t x)$$

It is analytic in the strip $\{0 < \operatorname{Im} z < 1\}$, continuous, and bounded on its closure. It follows that

$$\int dt\, F(t, s) = \int dt\, F(t+i, s)$$

Using this, the KMS property of the state ρ, and $f(t+i) = f(-t)$, one gets

$$\rho(y^*\Gamma_\rho y) = -\int dt\, ds\, f(s-t)\,\overline{\rho([\alpha_t x, y])}\,\rho([\alpha_s x, y]) \leqslant 0$$

because the function f is of positive type. ∎

The map Γ_ρ on $\mathscr{A}$ defines an operator, denoted by the same symbol, on the Hilbert space $\mathscr{H}_\rho$:

$$\Gamma_\rho(y\Omega_\rho) = \Gamma_\rho(y)\,\Omega_\rho; \qquad y \in \mathscr{A}_0 \tag{4.2}$$

Next we characterize completely this operator. For $x = x^* \in \mathscr{A}_0$, consider the function

$$\lambda \in \mathbb{R} \to \hat{F}^x_\rho(\lambda) = -\hat{f}(\lambda)(1-e^{-\lambda}) \int dt\, e^{-it\lambda} \rho([x, \alpha_t x]) \tag{4.3}$$

From the properties of f in (2.5) and the time invariance of ρ, it follows that

$$\overline{\hat{F}^x_\rho(\lambda)} = \hat{F}^x_\rho(-\lambda) = \hat{F}^x_\rho(\lambda)$$

If x has bounded spectral support, Proposition 2.4 implies that $\hat{F}_\rho^x$ is a negative bounded function. Then

$$\hat{F}_\rho^x(H_\rho) = \int \hat{F}_\rho^x(\lambda)\, dE_{-\lambda}$$

is a negative bounded operator on $\mathcal{H}_\rho$.

Again for $x = x^* \in \mathcal{A}_0 \subset \mathcal{M}_\rho$, define the subspace $\mathcal{H}_\rho^x$ of $\mathcal{H}_\rho$ generated by the vectors

$$\left\{ x(h)\, \Omega_\rho \mid x(h) = \int dt\, h(t)\, \alpha_t x;\, h \in L^1(\mathbb{R}) \right\} \tag{4.4}$$

Denote by P_ρ^x the corresponding orthogonal projection. Because

$$\alpha_s x(h) = x(h_s)$$

where h_s is the translate of h over s, the space $\mathcal{H}_\rho^x$ is time invariant, i.e.,

$$e^{isH_\rho} x(h)\, \Omega_\rho = \alpha_s x(h)\, \Omega_\rho = x(h_s)\, \Omega_\rho \in \mathcal{H}_\rho^x$$

and hence $[H_\rho, P_\rho^x] = 0$.

Lemma 4.2. Suppose that the observable $x = x^* \in \mathcal{A}_0$ has a bounded spectral support; then the operator Γ_ρ on $\mathcal{H}_\rho$ in (4.2) extends to a s.a. negative bounded operator explicitly given by

$$\Gamma_\rho = \hat{F}_\rho^x(H_\rho)\, P_\rho^x \tag{4.5}$$

Hence Γ_ρ is the generator of a contraction semigroup on $\mathcal{H}_\rho$, explicitly given by

$$\exp(t\Gamma_\rho) = (1 - P_\rho^x) + \{\exp[t\hat{F}_\rho^x(H_\rho)]\}\, P_\rho^x$$

Proof. (a) First we show that the range of Γ_ρ is contained in $\mathcal{H}_\rho^x$. Indeed, for all $y \in \mathcal{A}_0$, from (4.1) and (4.2),

$$\begin{aligned} \Gamma_\rho(y\Omega_\rho) &= \Gamma_\rho(y)\, \Omega_\rho \\ &= \int ds\, \rho([y, \alpha_s x(g)])\, \alpha_s x \Omega_\rho \end{aligned}$$

where $g(t) = f(t) - f(-t)$; $g \in L^1(\mathbb{R})$. As $x, y \in \mathcal{A}_0$, the function

$$s \to F_\rho^{x,y}(s) = \rho([y, \alpha_s x(g)]) \in L^1(\mathbb{R})$$

Hence $\Gamma_\rho(y\Omega_\rho) = x(F_\rho^{x,y})\,\Omega_\rho \in \mathscr{H}_\rho^x$ or

$$P_\rho^x \Gamma_\rho = \Gamma_\rho$$

(b) Take now $y = x(h)$ with $h \in L^1(\mathbb{R})$; then one computes

$$\Gamma_\rho(x(h)\,\Omega_\rho) = x(h * F_\rho^x)\,\Omega_\rho$$

(with $F_\rho^{x,x} \equiv F_\rho^x$), where $h * F_\rho^x$ is the convolution product of h and F_ρ^x, and therefore $h * F_\rho^x \in L^1(\mathbb{R})$. Using $f(t+i) = f(-t)$, one gets

$$\hat{g}(\lambda) = \hat{f}(\lambda)(1 - e^{-\lambda})$$

implying that indeed the function $\hat{F}_\rho^x$ defined by (4.3) is the Fourier transform of the function F_ρ^x introduced above. On the other hand, one more straightforward computation yields

$$\hat{F}_\rho^x(H_\rho)\,x(h)\,\Omega_\rho = x(h * F_\rho^x)\,\Omega_\rho = \Gamma_\rho x(h)\,\Omega_\rho$$

for all $h \in L^1(\mathbb{R})$.

As the observable x has a bounded spectral support, the above expression proves that Γ_ρ extends uniquely to the bounded operator $\hat{F}_\rho^x(H_\rho)$ on the invariant subspace $\mathscr{H}_\rho^x$.

(c) Using (a) and (b), i.e., $P_\rho^x\Gamma_\rho = \Gamma_\rho$ and the fact that Γ_ρ is a bounded operator on $\mathscr{H}_\rho^x$, one gets for all $y, z \in \mathscr{A}_0$

$$\begin{aligned}(y\Omega_\rho, \Gamma_\rho P_\rho^x z\Omega_\rho) &= (P_\rho^x \Gamma_\rho\, y\Omega_\rho, z\Omega_\rho)\\ &= (\Gamma_\rho\, y\Omega_\rho, z\Omega_\rho)\\ &= (y\Omega_\rho, \Gamma_\rho z\Omega_\rho)\end{aligned}$$

For the second equality we used Lemma 4.1(iii). This proves

$$\Gamma_\rho P_\rho^x = \Gamma_\rho = P_\rho^x \Gamma_\rho$$

or

$$\Gamma_\rho = P_\rho^x \Gamma_\rho P_\rho^x$$

and because of (b), Γ_ρ is a bounded operator given by

$$\Gamma_\rho = \hat{F}_\rho^x(H_\rho)\,P_\rho^x$$

It follows immediately that Γ_ρ is the generator of a contraction semigroup on $\mathscr{H}_\rho$. The explicit formula for the semigroup is a direct consequence of $[P_\rho^x, \hat{F}_\rho^x(H_\rho)] = 0$. ∎

Consider now the real vector space $\mathscr{H}_\rho^{\mathrm{Re}}$ of $\mathscr{H}_\rho$ generated by $\mathscr{A}_{0,\mathrm{sa}}\Omega_\rho$.

By continuity, the symplectic form σ_ρ of (2.1) and the positive bilinear form s of (2.3) extend to $\mathscr{H}_\rho^{\mathrm{Re}}$. They are explicitly given by

$$\sigma_\rho(\psi, \varphi) = -i((\psi, \varphi) - (\varphi, \psi))$$
$$s(\psi, \varphi) = \mathrm{Re}(\psi - (\Omega_\rho, \psi)\,\Omega_\rho, \varphi - (\Omega_\rho, \varphi)\,\Omega_\rho)$$

for $\psi, \varphi \in \mathscr{H}_\rho^{\mathrm{Re}}$.

Also, by continuity,

$$W(\mathscr{A}_{0,\mathrm{sa}}, \sigma_\rho)'' = W(\mathscr{H}_\rho^{\mathrm{Re}}, \sigma_\rho)''$$

where the bicommutant is taken in the GNS representation of the state ω_s. By Lemma 4.1(ii) one also has

$$\Gamma_\rho(\mathscr{H}_\rho^{\mathrm{Re}}) \subseteq \mathscr{H}_\rho^{\mathrm{Re}} \tag{4.6}$$

Now we are able to formulate the main result of this section.

Theorem 4.3. Suppose $x = x^* \in \mathscr{A}_0$ has a bounded spectral support. The contraction semigroup $\exp t\Gamma_\rho$ on $\mathscr{H}_\rho$ induces a dynamical semigroup $(\tau_t)_{t \geqslant 0}$ on the von Neumann algebra $W(\mathscr{H}_\rho^{\mathrm{Re}}, \sigma_\rho)''$; it is explicitly given by

$$\tau_t W(y) = W(e^{t\Gamma_\rho} y)\,\frac{\omega_s(W(y))}{\omega_s(W(e^{t\Gamma_\rho} y))}; \qquad y \in \mathscr{H}_\rho^{\mathrm{Re}}$$

The generator of τ_t is a self-adjoint extension of the symmetric map L_ρ, defined in Theorem 3.2.

Furthermore the semigroup τ_t satisfies the *Onsager relations*, i.e.,

$$\omega_s(W(y)\,\tau_t W(z)) = \omega_s(\tau_t(W(y))\,W(z))$$

for all $y, z \in \mathscr{H}_\rho^{\mathrm{Re}}$.

Proof. It follows from Lemma 4.2 that for all $t \geqslant 0$, the map

$$\tau_t\colon\quad W(y) \to \tau_t W(y) = W(e^{t\Gamma_\rho} y)\,\frac{\omega_s(W(y))}{\omega_s(W(e^{t\Gamma_\rho} y))}$$

is well defined. It follows from refs. 17 and 18 that $(\tau_t)_{t \geqslant 0}$ is a dynamical semigroup on the von Neumann algebra indicated above.

In order to show that L_ρ is the generator of the dynamical semigroup, we compute the weak operator topology derivative, using the symmetry of L_ρ and the formula

$$\omega_s(W(y)) = \exp -\tfrac{1}{2} s(y, y)$$

The result is

$$\frac{d}{dt}\tau_t W(y)|_{t=0} = [iB_\rho(\Gamma_\rho y) + s(\Gamma_\rho y, y)]\, W(y)$$

Using the computation in the proof of Lemma 4.1(v), one has $\chi_\rho(y) = s(\Gamma_\rho y, y)$.

Finally, the Onsager relations are easily established by an explicit computation using again the properties of Γ_ρ given in Lemma 4.2. This completes the proof of the theorem. ▮

As is well known,[1] the Onsager relations or Onsager's theorem are a macroscopic expression of the property of microscopic reversibility or the detailed balance property of the microsystem. In the literature the Onsager relations are mostly expressed in terms of the generator L_ρ of the macrosystem evolution τ_t. Normally, it is argued that the generator L_ρ is symmetric.[1,9] It is clear that L_ρ being symmetric is equivalent to $\tau_t = \exp tL_\rho$ being symmetric.

Here we get a rigorous proof of the Onsager relations starting from a microscopic model. We proved that the Onsager relations are in fact equivalent to the detailed balance property of L_ρ or τ_t with respect to the macroscopic system, given by the CCR-algebra of fluctuations of the microsystem, its equilibrium state ω_s, and its time evolution $\tilde{\alpha}_t$. The basic theorem for the transition from the microlevel to the macrolevel is of course the central limit theorem (3.2).

Furthermore, in connection with Theorem 4.3, remark that the irreversible evolution τ_t is completely determined by the map Γ_ρ acting on the space of thermal wave functions $\mathscr{H}_\rho$. In this context Lemma 4.2, formula (4.5) yields very detailed information about the spectrum of Γ_ρ. For various models the approach to equilibrium can be read off immediately from this explicit expression. We come back to this point in the next section.

5. ENTROPY PRODUCTION AND APPROACH TO EQUILIBRIUM

Above we arrived at a microscopic foundation of the macroscopic irreversible dynamics satisfying the Onsager relations. In this section we treat several other aspects of the irreversible dynamics, such as the approach to equilibrium and the related principle of minimal entropy production. For a physical introduction to these notions see refs. 1 and 9.

By the variational principle of statistical mechanics, an equilibrium state is characterized as a state minimizing the free energy density of the system. In phenomenological theories one considers a state "near to equilibrium" and looks for the increment in the free energy up to first approximation. As deviation from an extremum, the first approximation is a quadratic function in the perturbation. This is called the harmonic approximation or the linear response.

In the scheme developed above we have a mathematically rigorous understanding of the harmonic potential. First we describe states which are macroscopic but small perturbations of the equilibrium state.

Following Section 2, we consider again the microsystem $(\mathscr{A}, \rho, \alpha_t)$ and the macrosystem $(\mathscr{B}, \omega_\rho)$. For any $y \in \mathscr{A}_{\text{sa}}$ consider the perturbed state of $\mathscr{B}$ given by

$$\omega_\rho^{\tilde{y}^n}\left(\bigotimes_i a_i\right) = \prod_{j=1}^{n} \rho^{y/n}(a_i) \prod_{j>n} \rho(a_j); \qquad a_k \in \mathscr{A}_k$$

where $\rho^{y/n}$ is the equilibrium state for the perturbed Hamiltonian $H_\rho + y/\sqrt{n}$. In ref. 2 we proved the following result, which is a generalization of Theorem 2.1.

Theorem 5.1. For all $y, z \in \mathscr{A}_{\text{sa}}$ the limit

$$\lim_{n \to \infty} \omega_\rho^{\tilde{y}^n}(\exp i\tilde{z}^n)$$

exists and defines a quasifree state $\omega_{s,y}$ of the CCR-C^*-algebra of fluctuations $W(\mathscr{A}_{\text{sa}}, \sigma_\rho)$ such that

$$\lim_{n \to \infty} \omega_\rho^{\tilde{y}^n}(\exp i\tilde{z}^n) = \omega_{s,y}(W(z))$$

where

$$\omega_{s,y}(W(z)) = \omega_s(W(z)) \exp - i \int_0^1 du[\rho(z\alpha_{iu} y) - \rho(z)\, \rho(y)]$$

and

$$\omega_s(W(z)) = \exp - \tfrac{1}{2} s(z, z) \quad \blacksquare$$

Note that the sesquilinear map

$$(x, y)_\sim = \int_0^1 du\, \rho(x^* \alpha_{iu} y); \qquad x, y \in \mathscr{A}$$

is the well-known Duhamel two-point function or the so-called Bogoliubov scalar product. For a mathematical treatment of this quantity see ref. 19.

Remark also that all states of the type $\omega_{s,y}$ defined in Section 4.1 extend to the CCR-algebra $W(\mathscr{H}_\rho^{\mathrm{Re}}, \sigma_\rho)$. Denote by ξ_ρ the state space of all perturbed states of this type, i.e.,

$$\xi_\rho = \{\omega_{s,y} \mid y \in \mathscr{H}_\rho^{\mathrm{Re}}\} \tag{5.1}$$

This is the set of small perturbations of the equilibrium state ω_s of the fluctuations.

We prove that this class of perturbed states is invariant for the Onsager evolutions τ_t of Theorem 4.3.

Proposition 5.2. The set of states ξ_ρ is globally τ_t-invariant, in particular,

$$\omega_{s,y} \circ \tau_t = \omega_{s, e^{t\Gamma_\rho} y} \tag{5.2}$$

Proof. The proposition follows from the self-adjointness of Γ_ρ with respect to ρ and the fact that Γ_ρ commutes with the time evolution α_t (Lemma 4.2). Indeed, using the explicit formula of τ_t (Theorem 4.3), then

$$\begin{aligned}
&\omega_{s,y}(\tau_t W(z)) \\
&\quad = \omega_s(W(z)) \exp - i \int_0^1 du\, \rho\{(\exp t\Gamma_\rho)[z-\rho(z)]\, \alpha_{iu}[y-\rho(y)]\} \\
&\quad = \omega_s(W(z)) \exp - i \int_0^1 du\, \rho\{[z-\rho(z)]\, \alpha_{iu}(\exp t\Gamma_\rho)[y-\rho(y)]\} \\
&\quad = \omega_{s,e^{t\Gamma_\rho}y}(W(z)) \quad \blacksquare
\end{aligned}$$

Next we study the approach to equilibrium, i.e., we establish the existence of the limit

$$\lim_{t\to\infty} \omega_{s,y} \circ \tau_t$$

First we have a preparatory lemma, expressing that the set of zeros of the function $\hat{F}_\rho^x$ (Lemma 4.2) is small in the appropriate way. With the notation of Section 2 we have the following result.

Lemma 5.3. For $x = x^* \in \mathscr{A}_0$ with bounded spectral support Δ_x, denote $I_\rho^x = \{\lambda \in \mathbb{R} \mid \hat{F}_\rho^x(\lambda) = 0\}$; then for all $\psi \in \mathscr{H}_\rho^x$ [see (4.4)] with $(\psi, \Omega_\rho) = 0$ one has

$$\mu_\psi(I_\rho^x) = 0$$

Proof. First remark that $0 \in I_\rho^x$ and that for all $\psi \in \mathscr{H}_\rho^x$

$$\mu_\psi(\{0\}) = (\psi, E_\rho \psi) = (\psi, \Omega_\rho)(\Omega_\rho, \psi)$$

due to the ergodicity of ρ. Hence we have to prove that $\mu_\psi(I_\rho^x\backslash\{0\})=0$. For $\psi = x\Omega_\rho$ this is an immediate consequence of Proposition 2.4 and the regularity of the measure.

For $\psi = x(f)\,\Omega_\rho$, $f\in L^1(\mathbb{R}, dt)$, functional calculus yields

$$d\mu_{x(f)}(\lambda) = |\hat{f}(-\lambda)|^2\, d\mu_x(\lambda)$$

implying

$$\mu_{x(f)}(I_\rho^x\backslash\{0\}) \leqslant \|\hat{f}\|_\infty^2\, \mu_x(I_\rho^x\backslash\{0\}) = 0$$

For general $\psi\in\mathscr{H}_\rho^x$, there exists a sequence $\{f_n\}$, $f_n\in L^1(\mathbb{R}, dt)$, such that

$$\lim_n\,(\varphi, x(f_n)\,\Omega_\rho) = (\varphi, \psi) \qquad \text{for all} \quad \varphi\in\mathscr{H}_\rho$$

Hence

$$\begin{aligned}\mu_\psi(I_\rho^x\backslash\{0\}) &= (\psi, E_{I_\rho^x\backslash\{0\}}\psi)\\ &= \lim_{n\to\infty}\,(x(f_n)\,\Omega_\rho, E_{I_\rho^x\backslash\{0\}}x(f_n)\,\Omega_\rho)\\ &= \lim_{n\to\infty}\,\mu_{x(f_n)}(I_\rho^x\backslash\{0\})\\ &= 0 \quad \blacksquare\end{aligned}$$

Theorem 5.4. For all $x = x^*\in\mathscr{A}_0$ with bounded spectral support and for $\omega_{s,y}\in\xi_\rho$,

$$\lim_{t\to\infty}\,\omega_{s,y}\circ\tau_t = \omega_{s,(1-P_\rho^x)y}\in\xi_\rho$$

where the limit is taken in the weak *-topology.

Proof. (i) Consider first the case that $\rho(x)=0$. Then for all $f\in L^1(\mathbb{R}, dt)$

$$(\Omega_\rho, x(f)\,\Omega_\rho) = \hat{f}(0)(\Omega_\rho, x\Omega_\rho) = 0$$

Hence $P_\rho^x\Omega_\rho = 0$ and also $(\psi, \Omega_\rho)=0$ for $\psi = P_\rho^x\,y$, $y\in\mathscr{H}_\rho^{\mathrm{Re}}$.

By Lemma 5.3 and the regularity property of the measure μ_ψ, there exists a sequence of opens $(O_n)_n$ such that $I_\rho^x\subseteq O_n$ for all n and

$$\lim_{n\to\infty}\,\mu_\psi(O_n) = \mu_\psi(I_\rho^x) = 0$$

For all $\varphi \in \mathscr{H}_\rho$

$$|(\varphi, \{\exp[t\hat{F}^x_\rho(H_\rho)]\} P^x_\rho y)|^2 \leqslant (\varphi, \varphi)(P^x_\rho y, \exp[2t\hat{F}^x_\rho(H_\rho)] P^x_\rho y)$$
$$= (\varphi, \varphi) \int_{\Delta_\psi} \{\exp[2t\hat{F}^x_\rho(\lambda)]\}(\psi, dE_{-\lambda}\psi)$$

Take n large enough such that

$$\mu_\psi(O_n) < \frac{\varepsilon}{2(\varphi, \varphi)}$$

Using the negativity of the function $\hat{F}^x_\rho$, we obtain

$$|(\varphi, \{\exp[t\hat{F}^x_\rho(H_\rho)]\} P^x_\rho y)|$$
$$\leqslant \frac{\varepsilon}{2} + (\varphi, \varphi) \int_{\Delta_\psi \setminus O_n} \{\exp[2t\hat{F}^x_\rho(\lambda)]\}(\psi, dE_{-\lambda}\psi)$$

Because Δ_x is bounded and $\Delta_\psi \subseteq \Delta_x$, the set $\Delta_\psi \setminus O_n$ is compact in $\mathbb{R}$. The continuity of $\hat{F}^x_n$ implies that

$$\sup_{\lambda \in \Delta_\psi \setminus O_n} \hat{F}^x_\rho(\lambda) = -c_n < 0$$

For t large enough,

$$e^{-2tc_n}(y, y)(\varphi, \varphi) < \varepsilon/2$$

and

$$|(\varphi, \{\exp[t\hat{F}^x_\rho(H_\rho)]\} P^x_\rho y)|^2$$
$$\leqslant \frac{\varepsilon}{2} + (\varphi, \varphi)[\exp(-2tc_n)] \int_{\Delta_\psi \setminus O_n} (\psi, dE_{-\lambda}\psi)$$
$$\leqslant \frac{\varepsilon}{2} + (\varphi, \varphi)[\exp(-2tc_n)](P^x_\rho y, P^x_\rho y) < \varepsilon$$

Using Lemma 4.2, this shows the existence of the following limit:

$$\lim_{t \to \infty} [\exp(t\Gamma_\rho)]\, y$$
$$= (1 - P^x_\rho)\, y + \lim_{t \to \infty} \{\exp[t\hat{F}^x_\rho(H_\rho)]\} P^x_\rho y$$
$$= (1 - P^x_\rho)\, y$$

Together with (4.6), $y \in \mathscr{H}^{\mathrm{Re}}_\rho$ implies that $P^x_\rho y \in \mathscr{H}^{\mathrm{Re}}_\rho$.

Finally, together with Proposition 5.2, one has that for all $z \in \mathscr{H}_\rho^{\mathrm{Re}}$,

$$\lim_{t\to\infty} \omega_{s,y}(\tau_t^x W(z))$$

$$= \lim_{t\to\infty} \omega_{s,[\exp(t\Gamma_\rho^x)]y}(W(z))$$

$$= \omega_s(W(z)) \lim_{t\to\infty} \exp[-i(z-(\Omega_\rho, z)\,\Omega_\rho, [\exp(t\Gamma_\rho^x)]\, y-(\Omega_\rho, y)\,\Omega_\rho)_\sim]$$

$$= \omega_s(W(z)) \exp[-i(z-(\Omega_\rho, z)\,\Omega_\rho, (1-P_\rho^x)\, y-(\Omega_\rho, y)\,\Omega_\rho)_\sim]$$

$$= \omega_s(W(z)) \exp[-i(z-(\Omega_\rho, z)\,\Omega_\rho, (1-P_\rho^x)\, y-(\Omega_\rho, (1-P_\rho^x)\, y)\,\Omega_\rho)_\sim]$$

$$= \omega_{s,(1-P_\rho^x)y}(W(z))$$

(ii) The case $\rho(x)\neq 0$. As

$$E_\rho x \Omega_\rho = \rho(x)\,\Omega_\rho \in \mathscr{H}_\rho^x$$

one has $P_\rho^x \Omega_\rho = \Omega_\rho$.

Analogously as in the case (i), one shows that

$$\lim_{t\to\infty} [\exp(t\Gamma_\rho^x)]\; y = (1-P_\rho^x)\; y + (y, \Omega_\rho)\,\Omega_\rho$$

implying

$$P_\rho^x\, y \in \mathscr{H}_\rho^{\mathrm{Re}} \qquad \text{for all} \quad y \in \mathscr{H}_\rho^{\mathrm{Re}}$$

and for all y, $z \in \mathscr{H}_\rho^{\mathrm{Re}}$

$$\lim_{t\to\infty} \omega_{s,y}(\tau_t^x W(z)) = \omega_{s,(1-P_\rho^x)y}(W(z))$$

finishing the proof of the theorem. ∎

Clearly, this theorem describes in a detailed manner the approach to equilibrium. For a given $x \in \mathscr{A}_0$ all perturbations $\omega_{s,y}$ with $y \in \mathscr{H}_\rho^x$ are driven to the equilibrium ω_s of the fluctuations. If y belongs to the orthogonal complement, then the perturbed state is left unchanged. Hence the mechanism of the approach to equilibrium is seen very explicitly.

As far as the rate of convergence to equilibrium is concerned, this theorem does not give any information. For that one should analyze more carefully the set of zeros I_ρ^x of the function $\hat{F}_\rho^x$.

Finally, we turn to the notion of entropy production of the states $\omega_{s,y}$ under the irreversible dynamics τ_t. In ref. 2 we proved the following formula:

$$S(\omega_{s,y} \mid \omega_s) = -\tfrac{1}{2}(y-(y, \Omega_\rho)\,\Omega_\rho,\; y-(y, \Omega_\rho)\,\Omega_\rho)_\sim \tag{5.3}$$

for all $y \in \mathscr{H}_\rho^{\mathrm{Re}}$ and $\omega_{s,y} \in \xi_\rho$. In fact, we proved it for a dense set of elements y and then extend it by continuity. Furthermore, $S(\omega_{s,y} \mid \omega_s)$ stands for the relative entropy of $\omega_{s,y}$ with respect to ω_s defined in the frame of the Tomita–Takesaki theory.[11] The importance of this result (5.3) is situated not only in the existence of this relative entropy, but also in its explicit expression, being quadratic in the perturbation y.

Physically, the relative entropy (5.3) is shown[20] to be the increment in free energy due to a perturbation of the Hamiltonian by a fluctuation.

As usual, the entropy production of the state $\omega_{s,y}$ under the dynamics τ_t^x is defined by

$$\sigma_x(\omega_{s,y}) = \frac{d}{dt} S(\omega_{s,y} \circ \tau_t^x \mid \omega_s \circ \tau_t^x)|_{t=0}$$

We have the following result.

Theorem 5.5. For $x = x^* \in \mathscr{A}_{0,\mathrm{sa}}$ with bounded spectral support Δ_x, and for all $y \in \mathscr{H}_\rho^{\mathrm{Re}}$, the following hold:

(i) $\sigma_x(\omega_{s,y}) = -(\Gamma_\rho^x y, y)_\sim \geqslant 0.$

(ii) If $\sigma_x(\omega_{s,y}) = 0$ for all $x \in \mathscr{A}_{0,\mathrm{sa}}$, then $\omega_{s,y} = \omega_s$.

Proof. (i) Follows from Lemma 4.2, Proposition 5.2, and formula (5.3) by a direct computation.

(ii) Take any $x \in \mathscr{A}_{0,\mathrm{sa}}$ with $0 \notin \Delta_x$; then from the definition of the Duhamel two-point function, Proposition 5.2, and part (i), one computes

$$\begin{aligned}\sigma_x(\omega_{s,y}) &= -\int \frac{1 - e^{-\lambda}}{\lambda} (\Gamma_\rho^x y, dE_{-\lambda} y) \\ &= -\int_{\Delta_\psi} \frac{1 - e^{-\lambda}}{\lambda} \hat{F}_\rho^x(\lambda)\, d\mu_\psi(\lambda)\end{aligned}$$

where $\psi = P_\rho^x y$.

As $0 \notin \Delta_x$, one has that $\rho(x) = 0$, implying that $P_\rho^x \Omega_\rho = 0$ (see proof of Theorem 5.4). Hence $(\psi, \Omega_\rho) = 0$. From Lemma 5.3, $\hat{F}_\rho^x(\lambda) \neq 0$, μ_ψ-almost everywhere.

Hence, as $\hat{F}_\rho^x < 0$, $\sigma_x(\omega_{s,y}) = 0$ implies

$$0 = \int d\mu_\psi(\lambda) = (P_\rho^x y, P_\rho^x y) \qquad \text{or} \qquad P_\rho^x y = 0$$

But this holds for all $x \in \mathscr{A}_0$, $0 \notin \Delta_x$. Therefore

$$(x\Omega_\rho, y) = 0 \qquad \text{for all } x \text{ with } 0 \notin \Delta_x$$

From spectral theory, $y \in E_\rho \mathscr{H}_\rho$ and by ergodicity of the state ρ,

$$y = (\Omega_\rho, y)\, \Omega_\rho$$

and $\omega_{s,y} = \omega_s$. ∎

It is clear that also the entropy production of a perturbed state is again a quadratic expression in the perturbation y. The second statement of the theorem is the mathematical expression of the principle of minimal entropy production.

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