Detailed balance and quantum dynamical maps



1998 J. Phys. A: Math. Gen. 31 7981

(http://iopscience.iop.org/0305-4470/31/39/013)

J. Phys. A: Math. Gen. **31** (1998) 7981–7995. Printed in the UK PII: S0305-4470(98)92743-3

# Detailed balance and quantum dynamical maps

W A Majewski† and R F Streater‡

† Institute of Theoretical Physics, Gdańsk University, 88-952 Gdansk, Poland

‡ Department of Mathematics, King's College, The Strand, London WC2R 2LS, UK

Received 24 March 1998

**Abstract.** Let $T$ be a stochastic map on a $C^*$-algebra $\mathcal{A}$, and $\omega$ a faithful state. Let $\pi_\omega(T)$ be the induced action of $T$ on the GNS Hilbert space $\mathcal{H}_\omega$, and $\pi_\omega(T)^*$ its adjoint on $\mathcal{H}_\omega$. We say $T$ obeys detailed balance II if $\pi_\omega(T)^*$ is also induced by a stochastic map. In that case we prove that $\pi_\omega(T)$ is a contraction on $\mathcal{H}_\omega$ commuting with the modular operator. The relation of this idea to microscopic reversibility is discussed. An entropy estimate is presented.

## 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. We consider the case where $t = 0, 1, \ldots$ (discrete time). In this case the semigroup is the family of maps generated by a single stochastic map $T = T_1 : \mathcal{A} \to \mathcal{A}$. Thus $T_t$ obeys

(i) $T_t$ is positive: $T_t(A^*A) \geqslant 0$ for all $A \in \mathcal{A}$.
(ii) $T_t(1) = 1$.
(iii) $T_s \circ T_t = T_{s+t}$, $t, s \geqslant 0$.

By Størmer's theorem, each $T_t$ is a norm contraction [6, corollary 3.2.6].

The natural action $T_t^\flat$ on the dual space $\mathcal{A}^*$

$$T_t^\flat \varphi(A) = \varphi(T_t A) \qquad \varphi \in \mathcal{A}^* \quad A \in \mathcal{A} \tag{1}$$

maps the set of states $\Sigma(\mathcal{A}) \subset \mathcal{A}^*$ to itself. We shall be interested in a kind of inverse to this natural action; its existence is not clear unless we make further assumptions.

In non-equilibrium, isothermal quantum statistical mechanics we have a faithful state $\omega$, the equilibrium state at some $\beta$, invariant under $T_t^\flat$. The Gelfand–Naimark–Segal construction then gives us a representation $\pi_\omega$ of $\mathcal{A}$ on a Hilbert space $\mathcal{H}_\omega$, with cyclic vector $\Omega_\omega$, 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

$$\pi_\omega(T_t)\pi_\omega(A)\Omega_\omega = \pi_\omega(T_t A)\Omega_\omega. \tag{2}$$

The question arises as to whether $\pi_\omega(T_t)$ is bounded or even closable. This problem goes to the heart of Tomita–Takesaki theory. This important question was raised in [19, 20]; in the case of continuous time it was shown that $\pi_\omega(T_t)$ is a contraction under one further condition, which will be called detailed balance I, and which is related to the existence of a form of time-reversal for the underlying dynamics. For this reason, chemists [5] prefer the more accurate term 'microscopic reversibility' for this notion, reserving detailed balance for the original use of Tolman [28]. However, 'detailed balance' has permeated the literature in physics, and even mathematics, after the paper of Glauber [14], and we shall retain it. It is easy to check that when $T_t$ is an automorphism, then on states of $\mathcal{H}_\omega$, $\pi_\omega(T_t)$ corresponds to $T^\flat_{-t}$.

It is noteworthy that in [19, 20] it was not necessary to assume completely positivity of the maps $T_t$: this leads to an easy proof of the contractivity. This raises the question as to whether a similar result holds in the case of discrete time. Again, even two-positivity leads to a short proof, by Kadison's inequality [16]. In this paper we formulate the general condition, detailed balance II, in the form: $\pi_\omega(T)^*$ is induced from a stochastic map (denoted $T^\beta$). This implies that $\omega$ is a fixed point of $T^\flat$. In section 2 we show that detailed balance I implies detailed balance II, and that detailed balance II implies that $\pi_\omega(T_t)$ is a contraction in $\mathcal{H}_\omega$. This gives a shorter proof than in [19, 20], and also extends the result to discrete time. Inasmuch as detailed balance II is more general than detailed balance I (and we have no complete proof of this) the present result is more general than [19, 20]. The dynamics advocated in [24] are all projections of random conservative dynamics, and were shown to satisfy detailed balance II, as well as being completely positive.

In the classical case, in which the algebra is abelian, that $\omega$ is a fixed point of $T^\flat_t$ is sufficient for detailed balance II (see [25, lemmas 5.23 and 5.24]). This is not so in the quantum case, since as we show in section 2 there are stochastic maps $T$, even in two dimensions, for which $\pi_\omega(T)$ is not a contraction. This is traced to the fact that it is not Hermitian, i.e. it does not map the self-adjoint operators to themselves. We then show that if, in addition to being closable and having $\Omega_\omega$ as a fixed point, $\pi_\omega(T)^*$ is induced by a Hermitian map $T^\beta$, then $T^\beta$ is positive, and so is a stochastic map. In section 3 we discuss the relation between the two forms of detailed balance; the section ends with some entropy estimates.

## 2. Detailed balance and contractivity

Suppose that $T$ is a stochastic map on $\mathcal{A}$ and that $T^\beta$ is another related by

$$\langle \pi_\omega(A)\Omega_\omega, \pi_\omega(T)\pi_\omega(B)\Omega_\omega\rangle = \langle \pi_\omega(T^\beta)\pi_\omega(A)\Omega_\omega, \pi_\omega(B)\Omega_\omega\rangle \tag{3}$$

which from the definition gives

$$\omega(A^*T(B)) = \omega(T^\beta(A^*)B). \tag{4}$$

This condition, called detailed balance II, implies $T$-invariance of the state $\omega$:

$$\omega(T(A)) = \omega(1T(A)) = \omega(T^\beta(1)A) = \omega(A).$$

Since $T^\beta$ is positive, it is Hermitian, and since it is stochastic, it is a contraction in norm. Then

$$\begin{aligned}
\|\pi_\omega(T)\pi_\omega(A)\Omega_\omega\|^2 &= \omega(T(A^*)T(A)) = \omega(A^*T^\beta T(A)) \\
&\leqslant \omega(A^*A)^{1/2}\omega(T^\beta(TA))^*T^\beta(T(A)))^{1/2} \\
&= \omega(A^*A)^{1/2}\omega(A^*T^\beta(T(T^\beta(T(A)))))^{1/2} \\
&\leqslant \omega(A^*A)^{1/2}\omega(A^*A)^{1/4}\omega(T^\beta(T(T^\beta(TA^*)))T^\beta(T(T^\beta(T(A)))))^{1/4} \\
&\;\vdots \\
&\leqslant \omega(A^*A)^{1-1/2^n}\omega(T^\beta(T\cdots(A^*))T^\beta\cdots T(A))^{1/2^n}
\end{aligned}$$

for all $n$. Now

$$\omega(A^*A)^{1-2^{-n}} \to \omega(A^*A) \qquad \text{as } n \to \infty$$
$$|\omega(B^*B)|^{2^{-n}} \leqslant \|A\|^{2^{-(n-1)}} \to 1 \qquad \text{as } n \to \infty$$

where $B = T^\beta(T \cdots (A))$. Therefore, taking $n \to \infty$,

$$\|\pi_\omega(T)\pi_\omega(A)\Omega_\omega\|^2 \leqslant \omega(A^*A) = \|\pi_\omega(A)\Omega_\omega\|^2. \tag{5}$$

Thus we have proved

*Proposition 1.* Detailed balance II implies the contractivity of the induced map $\pi_\omega(T)$ on $\mathcal{H}_\omega$. □

There have been various versions of the detailed balance condition; apart from [19], one can mention [1, 4, 11, 12, 17, 15, 18]. These concern continuous time, and mostly require complete positivity; in [18], the Hamiltonian part of the Lindblad generator is taken to be the KMS Hamiltonian, an assumption that we do not need. Moreover, the assumption that the generator commutes with the modular operator, made in [1] and [15], is a result of our formulation, rather than a postulate. Neither do we need the generator to be a normal operator, as used in [17]. Agarwal's treatment is rigorous in finite dimensions, and has a special form for the time-reversal operator. Alicki's definition was given in finite dimensions, and requires normality of the generator; in [11] (an abstract version of [4]) normality is also required, which is not used here. Comparison of [17] with detailed balance I has been discussed in [20]; apart from complete positivity, [17] needs splitting the generator of the semigroup which is not required here.

We now give an example, in two dimensions, which shows that $T$ being stochastic with $\omega$ an invariant state is not enough to ensure that $\pi_\omega(T)$ is a contraction. Some condition like detailed balance II is needed for this; in our example, $T^\beta$ is not a Hermitian map, and this suggests that hermiticity rather than positivity might be enough; such an idea is indeed shown to be so.

*Example 2.* Let $\mathcal{A}$ be the algebra of all complex $2 \times 2$ matrices, and let $\omega_\lambda$ be the 'Powers' state with density matrix

$$\rho_\beta = \begin{pmatrix} \lambda & 0 \\ 0 & 1-\lambda \end{pmatrix} \qquad \lambda = (1 + \mathrm{e}^{-\beta})^{-1}.$$

The tracial state $\lambda = \frac{1}{2}$ corresponds to the infinite-temperature state $\beta = 0$. Consider the map

$$T(X) = T\begin{pmatrix} x_1 & x_2 \\ x_3 & x_4 \end{pmatrix} = \begin{pmatrix} x_1 & x_3 \\ x_2 & x_4 \end{pmatrix}.$$

It is well known [10] that $T$ is a linear, positive and identity-preserving map. It is not strongly positive; i.e.

$$T(A^*A) \geqslant T(A^*)T(A) \tag{6}$$

(Kadison's inequality [16]) does not hold.

Let us consider the natural action on the states

$$\langle T^\flat(\omega_\lambda), A\rangle = \mathrm{Tr}(\rho_\beta T(A)) = \mathrm{Tr}(\rho_\beta A^T)$$
$$= \mathrm{Tr}(\rho_\beta^T A) = \mathrm{Tr}(\rho_\beta A) = \omega_\lambda(A)$$

so $\omega_\lambda$ is a fixed point of $T^\flat$. For $\beta < \infty$, $\mathcal{H}_\omega$ is the space $\mathcal{A}$ with scalar product $\langle A, B\rangle = \mathrm{Tr}(A^*B)$ and cyclic vector $\rho_\beta^{1/2}$. Let us define

$$\pi_\beta(T)X\rho_\beta^{1/2} = T(X)\rho_\beta^{1/2}.$$

Then we see that

$$\|X\rho_\beta^{1/2}\|^2 = \omega_\lambda(X^*X) = \lambda(|x_1|^2 + |x_3|^2) + (1-\lambda)(|x_2|^2 + |x_4|^2)$$

whereas

$$\|T(X)\rho_\beta^{1/2}\|^2 = \lambda(|x_1|^2 + |x_2|^2) + (1-\lambda)(|x_3|^2 + |x_4|^2).$$

Now we cannot have

$$\lambda(|x_1|^2 + |x_2|^2) + (1-\lambda)(|x_3|^2 + |x_4|^2) \leqslant \lambda(|x_1|^2 + |x_3|^2) + (1-\lambda)(|x_2|^2 + |x_4|^2)$$

holding for all $x_2$, $x_3$, at least if $\lambda \neq \frac{1}{2}$. We conclude that $\pi_\beta(T)$ is not a contraction, and so that $T^\beta$ is not stochastic. A simple calculation shows that

$$T^\beta \begin{pmatrix} x_1 & x_2 \\ x_3 & x_4 \end{pmatrix} = \begin{pmatrix} x_1 & \left(\dfrac{1-\lambda}{\lambda}\right)x_3 \\ \left(\dfrac{\lambda}{1-\lambda}\right)x_2 & x_4 \end{pmatrix}.$$

We see that this is not a Hermitian map if $\lambda \neq 1/2$.

We now show that positivity can be replaced by hermiticity and a closability property. To explain our idea, let us recall the fundamental ingredients of Tomita–Takesaki theory. Consider a von Neumann algebra $\mathcal{M}$ on a Hilbert space $\mathcal{H}$ with a cyclic and separating vector $\Omega$. So, the state $\omega(A) = (\Omega, A\Omega)$, $A \in \mathcal{M}$ is faithful. Define

$$S_0 A\Omega = A^*\Omega \qquad A \in \mathcal{M} \tag{7}$$

and denote the closure of $S_0$ by $S$. Let $\Delta$ be the unique, positive, self-adjoint operator and $J$ the unique anti-unitary operator occurring in the polar decomposition

$$S = J\Delta^{1/2}. \tag{8}$$

$\Delta$ is called the modular operator associated with the pair $(\mathcal{M}, \Omega)$ and $J$ is called the modular conjugation (cf [6]). The following theorem can be extracted from the proof of [20, observation 3, theorem 3.10]:

*Theorem 3.* Let $T$ be a stochastic map on a von Neumann algebra $\mathcal{M}$ acting on a Hilbert space $\mathcal{K}_\omega$; let $\omega$ be a faithful vector state; let $\Omega \in \mathcal{K}_\omega$ be the (cyclic and separating) vector giving the state $\omega$, and define the operator $\hat{T}$ on the dense set $\mathcal{M}\Omega$ by

$$\hat{T}(A\Omega) = T(A)\Omega. \tag{9}$$

Suppose that $\hat{T}$ is closable. Let $\mathcal{M}_s$ be the set of self-adjoint elements of $\mathcal{M}$, and suppose that $\hat{T}^*$ maps $\mathcal{M}_s\Omega$ to itself. Then the closure of $\hat{T}$ commutes strongly with the modular operator on the domain $\mathcal{M}_s\Omega + \mathrm{i}\mathcal{M}_s\Omega$.

*Corollary 4.* Let $\mathcal{M}$ be a von Neumann algebra with cyclic and separating vector $\Omega$ and $T : \mathcal{M} \to \mathcal{M}$ a stochastic map on $\mathcal{M}$ obeying detailed balance II. Define $\hat{T}A\Omega = T(A)\Omega$. Then, $\hat{T}$ commutes strongly with the modular operator.

For $\hat{T}$ is a densely defined contraction, and so is closable; being positive, $T$ is Hermitian, and so maps the self-adjoint elements to themselves. The same holds for $\hat{T}^*$, determined by $T^\beta$, which is positive by detailed balance II. □

The next theorem is another immediate consequence of theorem 3.

*Proposition 5.* Let $\mathcal{M}$ be a von Neumann algebra on $\mathcal{H}$ with cyclic and separating vector $\Omega \in \mathcal{H}$ and $T : \mathcal{M} \to \mathcal{M}$ be a stochastic map. Assume that $T^\beta$ is a linear bounded Hermitian map on $\mathcal{M}$ such that

$$\langle A\Omega, T(B)\Omega\rangle = \langle T^\beta(A)\Omega, B\Omega\rangle. \tag{10}$$

Let $\hat{T} : \mathcal{H} \to \mathcal{H}$ be defined by

$$\hat{T} A\Omega = T(A)\Omega.$$

Then $\overline{\hat{T}}$ commutes strongly with the modular operator on the domain $\mathcal{M}_s\Omega + \mathrm{i}\mathcal{M}_s\Omega$.

*Proof.* $\hat{T^\beta} A\Omega = T^\beta(A)\Omega$ is a densely defined linear operator. Then

$$\langle \hat{T^\beta} A\Omega, B\Omega\rangle = \langle A\Omega, \hat{T} B\Omega\rangle = \langle \hat{T}^* A\Omega, B\Omega\rangle \qquad A, B \in \mathcal{M}. \tag{11}$$

Hence $\hat{T}^*$ is densely defined so $\hat{T}$ is a closable operator. Thus, another application of theorem 3 gives the commutativity of $\overline{\hat{T}}$ with the modular operator. □

In elementary quantum mechanics, $\mathcal{A} = \mathcal{B}(\mathcal{H})$ and $\omega$, a faithful normal state, is given by $\omega(\bullet) = \mathrm{Tr}(\varrho\bullet)$, where $\varrho$ is a density matrix on $\mathcal{H}$ with a densely defined inverse. For $\pi_\omega(A)$ we take left multiplication by $A$, with cyclic vector $\Omega = \varrho^{1/2}$, in the space $\mathcal{K}$ of all Hilbert–Schmidt operators on $\mathcal{H}$, with scalar product in $\mathcal{K} \equiv \mathcal{H}_{\text{H-S}}$ given by

$$\langle X, Y\rangle = \mathrm{Tr}(X^*Y) \qquad X, Y \in \mathcal{H}_\omega. \tag{12}$$

Thus

$$\pi_\omega(A)B\varrho^{1/2} = AB\varrho^{1/2} \qquad A, B \in \mathcal{A}. \tag{13}$$

Here and in the remainder of this section $\mathcal{M}$ will denote the von Neumann algebra on $\mathcal{K}$ generated by $\{\pi_\omega(A), A \in \mathcal{A}\}$.

The modular operator $\Delta$ and the modular conjugation are defined on the dense set $\mathcal{A}\varrho^{1/2}$ by

$$\Delta A\varrho^{1/2} = \varrho A\varrho^{-1/2} = \varrho A\varrho^{-1}\varrho^{1/2} \tag{14}$$

$$JA\varrho^{1/2} = \varrho A^*. \tag{15}$$

We see in particular that $\Delta^{1/2}A\Omega = \varrho^{1/2}A\varrho^{-1/2}\Omega$.

*Theorem 6.* Let $T$ be a normal† stochastic map on $\mathcal{B}(\mathcal{H})$ and $\omega$ a faithful normal state on $\mathcal{B}(\mathcal{H})$ such that $\omega \circ T = \omega$; let $\mathcal{K} = \mathcal{H}_\omega$ be the Gelfand–Naimark–Segal space and let $\varrho$ be the positive, invertible density matrix in $\mathcal{B}(\mathcal{H})$ corresponding to $\omega$. Assume that there exists a bounded Hermitian linear map $T^\beta$ on $\mathcal{B}(\mathcal{H})$ such that

$$\omega(BT(A)) = \omega(T^\beta(B)A) \qquad A, B \in \mathcal{M}. \tag{16}$$

Then $T^\beta$ is a stochastic map.

*Proof.* We first show that $T^\beta(1) = 1$. The T-invariance of $\omega$ and equation (16) imply

$$\begin{aligned}\langle T^\beta(1)^*\varrho^{1/2}, A\varrho^{1/2}\rangle &= \omega(T^\beta(1)A) = \omega(T(A)) = \omega(A)\\ &= \langle \varrho^{1/2}, A\varrho^{1/2}\rangle.\end{aligned}$$

Hence $T^\beta(1)\varrho^{1/2} = \varrho^{1/2}$, so as $\varrho^{1/2}$ is separating for $\mathcal{M}$, we have $T^\beta(1)^* = T^\beta(1) = 1$.

To prove the positivity of $T^\beta$, let $T^\dagger$ be the infinite-temperature conjugation, i.e.

$$\mathrm{Tr}(A^*T(B)) = \mathrm{Tr}(T^\dagger(A^*)B) \qquad \text{for all } A \text{ of trace class and } B \in \mathcal{B}(\mathcal{H}). \tag{17}$$

† That is, ultrastrongly continuous.

Thus, $T^\dagger$ is the restriction of $T^\flat$ defined in (1) to the density matrices, and so is positive (as $T$ is positive), and for $A, B \in \mathcal{B}(\mathcal{H})$

$$\begin{aligned}\mathrm{Tr}\left(\varrho T^\beta(B)A\right) &= \omega\left(T^\beta(B)A\right) = \omega\left(BT(A)\right) = \mathrm{Tr}\left(\varrho BT(A)\right)\\ &= \mathrm{Tr}\left(T^\dagger(\varrho B)A\right) \qquad \text{for all } A.\end{aligned}$$

Hence

$$T^\dagger(\varrho B) = \varrho T^\beta(B) \qquad \text{for all } B. \tag{18}$$

As $T : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ uniquely defines a map on $\mathcal{M}$, we shall denote the latter by the same symbol. Next, we observe that the commutativity of $\hat{T}$ with the modular operator (proposition 5) implies the commutativity of $T$ with the modular automorphism $\alpha_t(\bullet) = \Delta^{\mathrm{i}t} \bullet \Delta^{-\mathrm{i}t}$. Moreover, a calculation shows that the modular group is given by

$$\alpha_t(\cdot) = \varrho^{\mathrm{i}t} \cdot \varrho^{-\mathrm{i}t}.$$

This fact, the definition of $T^\dagger$ and the implementability of $\alpha_t$, give the commutativity of $T^\dagger$ with $\alpha_t$; to see this, let $A \in \mathcal{B}(\mathcal{H})$ and let $B$ be of trace class. Then

$$\begin{aligned}\mathrm{Tr}(\alpha_t T^\dagger(B)A) &= \mathrm{Tr}(T^\dagger(B)\alpha_{-t}(A)) = \mathrm{Tr}\left(BT(\alpha_{-t}(A))\right)\\ &= \mathrm{Tr}\left(B\alpha_{-t}T(A)\right) = \mathrm{Tr}\left(\alpha_t(B)T(A)\right)\\ &= \mathrm{Tr}\left(T^\dagger(\alpha_t(B))A\right).\end{aligned}$$

Since this holds for all $A$, we have

$$\alpha_t T^\dagger(B) = T^\dagger(\alpha_t(B)). \tag{19}$$

We shall use this equation for certain complex $t$; to justify this, note again that $\alpha_t$ is implemented by $\varrho^{\mathrm{i}t} \cdot \varrho^{-\mathrm{i}t}$; then equation (19) gives

$$\varrho^{\mathrm{i}t} T^\dagger(B)\varrho^{-\mathrm{i}t} = T^\dagger(\varrho^{\mathrm{i}t} B\varrho^{-\mathrm{i}t}). \tag{20}$$

We are interested in $B$ of the form $B = \varrho^{1/2}A\varrho^{1/2}$, $A \in \mathcal{B}(\mathcal{H})$. For such elements an analytic continuation $t \to z = t + \mathrm{i}s$ of $\mathrm{e}^{\mathrm{i}t}B\mathrm{e}^{-\mathrm{i}t}$ into the strip $-\frac{1}{2} \leqslant s \leqslant \frac{1}{2}$ is possible; for the proof, note that

$$\varrho^{\mathrm{i}t-s}\varrho^{1/2}A\varrho^{1/2}\varrho^{-\mathrm{i}t+s} = \varrho^{\mathrm{i}t}\left(\varrho^{1/2-s}A\varrho^{1/2+s}\right)\varrho^{-\mathrm{i}t}$$

is of trace class, so $\varrho^{1/2}A\varrho^{1/2}$ is an analytic element in this strip, and such a set is invariant under $T^\dagger$, as this commutes with $\alpha_t$. So the left-hand side of equation (19) has an analytic continuation into the strip. Putting $s = -\frac{1}{2}$ gives

$$\varrho^{1/2}T^\dagger(B)\varrho^{-1/2} = T^\dagger\left(\varrho^{1/2}B\varrho^{-1/2}\right) \tag{21}$$

for $B$ of the form $B = \varrho^{1/2}A\varrho^{1/2}$ giving

$$\varrho^{1/2}T^\dagger\left(\varrho^{1/2}A\varrho^{1/2}\right)\varrho^{-1/2} = T^\dagger(\varrho A) = \varrho T^\beta(A) \tag{22}$$

by equation (18). Hence

$$T^\beta(A) = \varrho^{-1/2}T^\dagger\left(\varrho^{1/2}A\varrho^{1/2}\right)\varrho^{-1/2} \tag{23}$$

and so is positive if $A$ is positive. Thus we have proved theorem 6. □

In the classical case the positivity of $T^\beta$ follows from that of $T$, as remarked in [25, lemma 5.24]. In the quantum case, our counterexample shows that this fails, but this theorem shows that we can replace detailed balance II by the conditions that $T^\beta$ is a Hermitian map and $\omega$ is invariant under $T$.

## 3. Relationships between two forms of detailed balance

In [19] the following condition, detailed balance I, was introduced; it involves the concept of microscopic reversibility, which was expressed thus: there exists an anti-linear Jordan automorphism $\sigma$ of $\mathcal{A}$ of order two (i.e. $\sigma^2 = \mathrm{id}$) such that

$$\omega(\sigma(A)\sigma(B)) = \omega(\sigma(AB)) \qquad \text{for} \quad A, B \in \mathcal{A} \tag{24}$$

and

$$\omega(A^*B) = \omega\left(\sigma(B^*)\sigma(A)\right). \tag{25}$$

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

$$\omega\left(A^*T(B)\right) = \omega\left(\sigma(B^*)T(\sigma(A))\right). \tag{26}$$

It will become clear that detailed balance I implies detailed balance II; this will be expressed in theorem 7. In addition, detailed balance I implies that there exists a basis in the representation space $\mathcal{H}_\omega$ in which $\pi(T)$ is symmetric (in the sense of (27) below). It seems to be impossible to derive this property from detailed balance II, leading us to believe that II is a properly weaker condition than I. In the case of a theory with a finite number of degrees of freedom, we shall consider a similar but more detailed condition which together with detailed balance II implies detailed balance I (see theorem 10 in section 3.2). For the rest of this section we shall consider the system described by a pair $(\mathcal{A} = \mathcal{B}(\mathcal{H}), \omega)$, as in equations (12)–(15), and a stochastic map $T$ on $\mathcal{A}$. We start with the easy direction.

### *3.1. Consequences of detailed balance I*

*Theorem 7.* Supppose that $T$ obeys detailed balance I, equation (26) relative to a time-reversal $\sigma$. Then $T$ obeys detailed balance II and in addition there exists a basis $\{y_i\}$ of $\mathcal{H}_{\text{H-S}}$ such that $\pi_\omega(T)$ is symmetric (not Hermitian) in this basis, i.e.

$$T_{k\ell} = \langle y_k, \pi_\omega(T)y_\ell\rangle = \langle y_\ell, \pi_\omega(T)y_k\rangle = T_{\ell k}. \tag{27}$$

*Proof.* From equation (26) we have

$$\begin{aligned}\omega(A^*T(B)) &= \omega\left(\sigma(B^*)T\sigma(A)\right)\\ &= \omega\left(\sigma(B^*)\sigma(\sigma \circ T \circ \sigma(A)\right)\end{aligned}$$

and by (25)

$$\omega(A^*T(B)) = \omega\left(\sigma \circ T \circ \sigma(A^*)B\right).$$

Therefore the adjoint $T^\beta$ relative to the KMS scalar product coincides with the stochastic map $\sigma \circ T \circ \sigma$, and so $T$ obeys detailed balance II.

We now construct the basis in which $\pi_\omega(T)$ is symmetric. Indeed, the operator $\mathcal{J}$ defined by

$$\mathcal{J}A\varrho^{1/2} = \sigma(A)\varrho^{1/2} \tag{28}$$

defines a conjugation on $\mathcal{H}_{\text{H-S}}$, a separable Hilbert space. Therefore there exists a real basis $\{y_j\}$, i.e. a basis with

$$\mathcal{J}y_j = y_j \qquad \text{for} \quad j = 1, 2, \ldots. \tag{29}$$

Then from equation (26) we have

$$\langle A\varrho^{1/2}, \pi_\omega(T)B\varrho\rangle = \langle \mathcal{J}B\varrho^{1/2}, \pi_\omega(T)\mathcal{J}A\varrho^{1/2}\rangle \tag{30}$$

and for the real basis

$$\langle y_k, \pi_\omega(T) y_\ell \rangle = \langle y_\ell, \pi_\omega(T) y_k \rangle \tag{31}$$

which proves the theorem. □

It turns out that because of the multiplicity of the eigenvalue 1 of $\Delta$ we are unable to be more specific about $\{y_k\}$; in particular, we cannot prove that every dyad associated with the spectral resolution of $\varrho$ can be chosen to be real (see the next topic).

### *3.2. Consequences of detailed balance II*

To get some kind of converse to theorem 7, denote by $\{x_i\}$ a basis in $\mathcal{H}$ of the eigenvectors of $\varrho$ (the density matrix of $\omega$). This basis is not determined uniquely; for example, we can change the phases. We define the conjugation $K$ by

$$Kf = K \sum_i (x_i, f) x_i = \sum_i \overline{(x_i, f)} x_i \tag{32}$$

for $f \in \mathcal{H}$, so that the basis is *real* relative to $K$. It is easy to observe that

(i) $K$ is a well-defined conjugation on $\mathcal{H}$,
(ii) the map

$$\mathcal{H}_{\text{H-S}} \ni \rho \mapsto K\rho K \equiv \mathcal{J}(\rho) \in \mathcal{H}_{\text{H-S}} \tag{33}$$

defines a conjugation $\mathcal{J}$ on $\mathcal{H}_{\text{H-S}}$.

We note that $\varrho$ is a real vector in this basis, so that $\mathcal{J}\varrho^{1/2} = \varrho^{1/2}$. Without trouble we can define an operator $A$ on $\mathcal{H}$ to be real if $A = KAK$. Extended to complex combinations of real operators we have an antilinear map $\sigma$ acting on $\mathcal{A} = \mathcal{B}(\mathcal{H})$. Let $V_0$ be the positive cone of the representation, i.e.

$$V_0 = \left\{ \pi_\omega(A)\varrho^{1/2}; \quad A \in \mathcal{B}(\mathcal{H}), \quad A \geqslant 0 \right\}. \tag{34}$$

Then $\mathcal{J}V_0 \subseteq V_0$, for

$$\begin{aligned} \mathcal{J}\pi_\omega(A^*)\pi_\omega(A)\varrho^{1/2} &= \mathcal{J}\pi_\omega(A^*)\mathcal{J}\mathcal{J}\pi_\omega(A)\mathcal{J}\varrho^{1/2} \\ &= \pi_\omega(\sigma(A^*A))\varrho^{1/2} \in V_0. \end{aligned} \tag{35}$$

Consequently, we can extend $\sigma$ to a reversing operation on $\pi_\omega(\mathcal{A})''$, i.e. $\sigma$ is an antilinear Jordan automorphism of order two, of the von Neumann algebra generated by the representation. (cf [20, lemma 4.11]). Define the operators of rank one on $\mathcal{H}_{\text{H-S}}$ by

$$(\overline{x} \otimes y) f = (x, f) y \qquad \text{for } x, y, f \in \mathcal{H}. \tag{36}$$

The inner product is taken to be linear in the second factor. Then the family $\{\overline{x} \otimes y\}$ form an orthonormal basis in $\mathcal{H}_{\text{H-S}}$ [27]. We note that $(\overline{x} \otimes y)^* = \overline{y} \otimes x$. Then

$$\varrho = \sum_n \lambda_n P_n = \sum_n \lambda_n (\overline{x}_n \otimes x_n). \tag{37}$$

Now let us define the operator $E_{ij} : \mathcal{H}_{\text{H-S}} \to \mathcal{H}_{\text{H-S}}$ by

$$E_{ij}\rho = P_i \rho P_j.$$

This is a projection, and $E_{ij}E_{k\ell} = 0$ unless $i = k$ and $j = \ell$. Thus

$$\Delta = \sum_{ij} \lambda_i^{-1} \lambda_j E_{ij}$$

is the spectral resolution of the modular operator, with eigenvalues $E_{ij} = \lambda_i^{-1}\lambda_j$ and spectral projection

$$Q_{E} = \sum_{i,j:E_{ij}=E} E_{ij}.$$

The action of $\Delta$ on $\mathcal{H}_{\text{H-S}}$ is

$$\Delta\rho = \sum_{ij} \lambda_i^{-1}\lambda_j P_i \rho P_j.$$

Obviously

$$\mathcal{J}\Delta(\rho) = \Delta(\mathcal{J}\rho).$$

We now give a lemma which explains the algebraic content of the proposed converse to theorem 7.

*Definition 8.* Let us denote

$$\omega_{ij,k\ell} = \omega\left(\overline{x}_j \otimes x_i T(\overline{x}_k \otimes x_\ell)\right) \tag{38}$$

$$\omega^{\beta}_{ij,k\ell} = \omega\left(\overline{x}_j \otimes x_i T^{\beta}(\overline{x}_k \otimes x_\ell)\right) \tag{39}$$

and

$$\tau_{ij,k\ell} = \langle \overline{x}_i \otimes x_j, \pi_\omega(T)\overline{x}_k \otimes x_\ell \rangle \tag{40}$$

$$\tau^{\beta}_{ij,k\ell} = \langle \overline{x}_i \otimes x_j, \pi_\omega(T^{\beta})\, \overline{x}_k \otimes x_\ell \rangle. \tag{41}$$

*Lemma 9.* Let $T$ satisfy detailed balance II; then we have

$$\tau_{ij,k\ell} = (\lambda_i\lambda_k)^{-1/2}\omega_{ij,k\ell} \tag{42}$$

$$\tau^{\beta}_{ij,k\ell} = (\lambda_i\lambda_k)^{-1/2}\omega^{\beta}_{ij,k\ell}. \tag{43}$$

*Proof.* By proposition 1, $\pi_\omega(T)$ and its adjoint are bounded. We see

$$\begin{aligned}
\tau_{ij,k\ell} &= \langle \overline{x}_j \otimes x_i, \pi_\omega(T)\, \overline{x}_k \otimes x_\ell \rangle = \mathrm{Tr}\big(\overline{x}_j \otimes x_i \cdot \pi_\omega(T)\lambda_k^{-1/2}\overline{x}_k \otimes x_\ell \varrho^{1/2}\big) \\
&= \mathrm{Tr}\, \overline{x}_j \otimes x_i \cdot T(\lambda^{-1/2}\overline{x}_k \otimes x_\ell)\varrho^{1/2} \\
&= \mathrm{Tr}\, \varrho^{1/2}\lambda_i^{-1/2}\overline{x}_j \otimes x_i \cdot T(\lambda_k^{-1/2}\overline{x}_k \otimes x_\ell)\varrho^{1/2} \\
&= (\lambda_i\lambda_k)^{-1/2}\omega_{ij,k\ell}.
\end{aligned}$$

A similar argument proves the second part. □

We are now ready to impose a further condition on a stochastic map $T$ which, with detailed balance II, implies detailed balance I. We say that $T$ is *effectively symmetric* if there exists a choice of phase of the eigenvectors $x_i$, $i = 1, 2, \ldots$ such that

$$\tau_{ij,k\ell} = \tau_{k\ell,ij} \qquad \text{for all } i, j, k, \ell. \tag{44}$$

*Theorem 10.* Let $T$ be a stochastic map that obeys detailed balance II relative to a normal state $\omega$ and suppose that $T$ is effectively symmetric. Then $T$ obeys detailed balance I relative to $\omega$ and the time-reversal given by $\sigma$ coming from equation (33).

*Proof.* By detailed balance II, $\pi_\omega(T)$ is a bounded operator. The reversing operation $\sigma$ has the property that $\overline{x}_i \otimes x_j$ are real. By lemma 9, and the fact that $\lambda_j$ is real for all $j$, we see that $\omega$ is effectively symmetric:

$$\omega_{ij,k\ell} = \omega_{k\ell,ij}. \tag{45}$$

This can be written as

$$\omega(A^* T(B)) = \omega(B^* T(A)) = \omega(\sigma(B^*) T \sigma(A)) \tag{46}$$

where $A = \overline{x}_i \otimes x_j$ and $B = \overline{x}_k \otimes x_\ell$. This is the condition for detailed balance I, equation (26) for dyads. Both sides are sesquilinear, and can be extended to the complex span of the dyads; any element $C$ of $\mathcal{A}$ is the strong$^*$ limit (in $\mathcal{H}$) of sums of dyads, and as $A_n \to C$ strongly, $A_n \varrho^{1/2} \to C \varrho^{1/2}$ in $\mathcal{H}_\omega$. Since the scalar product is continuous in this topology, and $\pi_\omega(T)$ is a bounded operator, we have proved detailed balance I in the form of (26). □

*Remarks 11.* Under the conditions of the theorem, one can show the following.

(i) $\sigma$ commutes with $T + T^\beta$, the dissipative part, and anticommutes with $(T - T^\beta)$, and so also commutes with the Hamiltonian part.
(ii) We also have

$$\overline{\tau}_{ij,k\ell} = \tau^\beta_{ij,k\ell}. \tag{47}$$

(iii) Consider a uniformly continuous semigroup of linear operators $\tau_t = \mathrm{e}^{tA}$ on a Hilbert space $\mathcal{K}$. Then, the symmetry of $\tau_t$ in some fixed basis implies the symmetry of the infinitesimal generator $A$ in the same basis. Next, the symmetry of $A_{mn}$ is equivalent to the compatibility of the decomposition $A$ into Hamiltonian and dissipative part ($A = \mathrm{i}H + D$) with the decomposition of $A_{mn}$ into real and imaginary parts.
To present an example of a semigroup satisfying equation (44) let us consider a self-adjoint operator

$$H = \sum_n \lambda_n \overline{x_n} \otimes x_n$$

where $\{x_n\}$ is some fixed CONS in $\mathcal{K}$, and a real symmetric matrix $D_{mn}$. Then define the semigroup $\tau_t = \mathrm{e}^{tA}$ by fixing the infinitesimal generator

$$A \equiv \mathrm{i}H + D = \mathrm{i} \sum_n \lambda_n \overline{x_n} \otimes x_n + \sum_{mn} D_{mn} \overline{x_n} \otimes x_m.$$

Clearly, $\tau_t$ satisfies (44) and generally $H$ does not commute with $D$.
(iv) The condition $T = T^\beta$ (which is often used, and is obviously much stronger that detailed balance II) implies that $\omega_{ij,k\ell}$ is Hermitian rather than symmetric. It does not seem to be connected with microscopic reversibility, i.e. the existence of a reversing operator $\sigma$. Rather, it expresses the vanishing of the Hamiltonian part, $\mathrm{i}(T - T^\beta)$ of the dynamics. Models constructed by projections of random reversible dynamics [25] do not in general obey this hermiticity condition.
(v) Either hermiticity or symmetry implies

$$|\omega_{ij,kl}|^2 = |\omega_{kl,ij}|^2 \tag{48}$$

which is Pauli's form of the detailed balance.

*3.3. Dual norms*

In [24, 26] and [25, theorem 5.33], the use of the dual KMS-norms in the study of Markov chain was described. In particular, it was shown that estimates of the relative entropy play a crucial role in the description of the states close to equilibrium. We want to close this section with a relation between the relative entropy in the quantum case and the dual KMS-norms, but in the opposite direction from that of [24] and [26]. The norm dual to that given by the Kubo–Martin–Schwinger construction (cf [24]) can be defined as

$$\|\nu\|_{-\beta} = \sup_{\|A\|_\beta \leqslant 1} |\nu(A)| \tag{49}$$

where $\nu$ is a state on $\mathcal{B}(\mathcal{H})$, $\|A\|_\beta^2 = \omega(A^*A)$, and $\omega(\cdot) = \operatorname{Tr}\varrho(\cdot)$ is the given faithful state on $\mathcal{B}(\mathcal{H})$. Let $\omega'(\cdot) = \operatorname{Tr}\varrho'(\cdot)$ be another faithful normal state on $\mathcal{B}(\mathcal{H})$. Then

$$\Delta_{\omega,\omega'} = \varrho' J \varrho^{-1} J$$

is the relative modular operator for the pair $(\pi_\omega(\mathcal{B}(\mathcal{H})), \varrho^{1/2})$. We shall assume that $\varrho^{1/2}$ is in the domain of $\Delta_{\omega,\omega'}$. To avoid future confusion let us emphasize that $J$ stands for the modular conjugation while $\mathcal{J}$ stands for the conjugation induced by the reversing operation. In general, $J \neq \mathcal{J}$.

A straightforward calculation gives

$$\|\omega'\|_{-\beta} = \|\Delta_{\omega,\omega'}\varrho^{1/2}\|_\beta \qquad \left(= \sup_{\|A\|_\beta \leqslant 1} |(\varrho^{1/2}\Delta_{\omega,\omega'}A\varrho^{1/2})|\right).$$

The relative entropy $S(\omega, \omega')$ can be defined as (cf [2, 3, 22])

$$S(\omega,\omega') = (\varrho^{1/2}, \log \Delta_{\omega,\omega'}\varrho^{1/2}) \qquad (= \operatorname{Tr}\varrho^{1/2} \log \Delta_{\omega,\omega'}\varrho^{1/2}).$$

*Lemma 12.*

$$O \geqslant S(\omega,\omega') \geqslant -\|f(\Delta_{\omega,\omega'}^{1/2})\varrho^{1/2}\|\,\|\omega - \omega'\|_{-\beta} \tag{50}$$

where

$$f(x) = \begin{cases} -1 & \text{if } x \geqslant 1 \\ x^{-1} & \text{if } 0 < x < 1. \end{cases}$$

*Proof.* Define the function $F(x) = f(x)(x^2 - 1)$. Clearly, $\log x \geqslant F(x)$. Hence

$$\begin{aligned} O \geqslant S(\omega,\omega') &= 2(\varrho^{1/2}, \log \Delta_{\omega,\omega'}^{1/2}\varrho^{1/2}) \geqslant (\varrho^{1/2}, F(\Delta_{\omega,\omega'}^{1/2})\varrho^{1/2}) \\ &\geqslant -|(\varrho^{1/2}, F(\Delta_{\omega,\omega'}^{1/2})\varrho^{1/2})| \\ &\geqslant -\|f(\Delta_{\omega,\omega'}^{1/2})\varrho^{1/2}\|\,\|(\Delta_{\omega,\omega'} - 1)\varrho^{1/2}\| \\ &= -\|f(\Delta_{\omega,\omega'}^{1/2})\varrho^{1/2}\| \sup_{\|\pi_\omega(A)\varrho^{1/2}\| \leqslant 1} |((\Delta_{\omega,\omega'} - 1)\varrho^{1/2}, \pi_\omega(A)\varrho^{1/2})| \\ &= -\|f(\Delta_{\omega,\omega'}^{1/2})\varrho^{1/2}\| \sup_{\|\pi_\omega(A)\varrho^{1/2}\| \leqslant 1} |(\Delta_{\omega,\omega'}\varrho^{1/2}, \pi_\omega(A)\varrho^{1/2}) - (\varrho^{1/2}, \pi_\omega(A)\varrho^{1/2})| \\ &= -\|f(\Delta_{\omega,\omega'}^{1/2})\varrho^{1/2}\| \sup_{\|\pi_\omega(A)\varrho^{1/2}\| \leqslant 1} |(\omega'(A) - \omega(A)| \\ &= -\|f(\Delta_{\omega,\omega'}^{1/2})\varrho^{1/2}\| \sup_{\|A\|_\beta \leqslant 1} |(\omega'(A) - \omega(A)| \\ &= -\|f(\Delta_{\omega,\omega'}^{1/2})\varrho^{1/2}\|\,\|\omega - \omega'\|_{-\beta} \end{aligned}$$

for states $\omega'$ such that $\varrho^{1/2}$ is in the domain of $\Delta_{\omega,\omega'}^{1/2}$. □

To prove the boundedness of $\| f(\Delta^{\frac{1}{2}}_{\omega,\omega'})\varrho^{1/2}\|$ we shall need

*Lemma 13 (Powers, Størmer).* Let $A$ and $B$ be positive operators on a Hilbert space $K$. Then

$$||A^{\frac{1}{2}} - B^{\frac{1}{2}}||^2_{\text{H-S}} \leqslant ||A - B||_{\text{T}} \tag{51}$$

where $||S||_{\text{H-S}}$ and $||S||_{\text{T}}$ denote the Hilbert–Schmidt and trace norms, respectively.

*Lemma 14.* Let $\varrho^{1/2}$ be in the domain of $\Delta^{-1/2}_{\omega,\omega'}$. Then

$$\{\| f(\Delta^{1/2}_{\omega,\omega'})\varrho^{1/2}\|\} \tag{52}$$

is bounded for $\omega \to \omega'$ in $\beta$-norm, i.e. for $\omega$ and $\omega'$ such that $\|\omega - \omega'\|_{-\beta} \to 0$.

*Proof.* Let us remark that

$$\begin{aligned}\|\omega - \omega'\|_{-\beta} &= \sup_{\|\pi_\omega(A)\varrho^{1/2}\|\leqslant 1} |(\omega'(A) - \omega(A)| \\ &\geqslant \sup_{\|A\|\leqslant 1} |(\omega'(A) - \omega(A)| \\ &= \sup_{\|A\|\leqslant 1} |\operatorname{Tr}\{\varrho' A\} - \operatorname{Tr}\{\varrho A\}| \\ &= ||\varrho' - \varrho||_{\text{T}}.\end{aligned}$$

Hence $\|\omega - \omega'\|_{-\beta} \to 0$ implies $\varrho \to \varrho'$ (in the trace norm). An application of lemma 13 leads to $(\varrho)^{1/2} \to (\varrho')^{1/2}$ (in the Hilbert–Schmidt norm $\|\cdot\|_{\text{H-S}} \equiv \|\cdot\|$). The next observation is

$$\begin{aligned}&\|\Delta^{1/2}_{\omega',\omega} x(\varrho')^{1/2} - \Delta^{1/2}_{\omega'} x(\varrho')^{1/2}\| = \|J\Delta^{1/2}_{\omega',\omega} x(\varrho')^{1/2} - J\Delta^{1/2}_{\omega'} x(\varrho')^{1/2}\| \\ &\qquad = \|x^*\varrho^{1/2} - x^*(\varrho')^{1/2}\| \leqslant \|x\|_\infty \|\varrho^{1/2} - (\varrho')^{1/2}\| \leqslant \|x\|_\infty \|(\varrho')^{1/2} - \varrho^{1/2}\|_{\text{T}}\end{aligned}$$

where $\|\cdot\|_{\text{T}}$ stands for the trace norm, $x \in \pi_\omega(\mathcal{B}(\mathcal{H}))$, $\|\cdot\|_\infty$ denotes the norm of the algebra $\pi_\omega(\mathcal{B}(\mathcal{H}))$, and $\Delta_\omega$ denotes the modular operator associated with the pair $(\pi_\omega(\mathcal{B}(\mathcal{H})), \varrho^{1/2})$. Consequently, the condition $\|\omega' - \omega\|_{-\beta} \to 0$ implies $\Delta^{1/2}_{\omega',\omega} \to \Delta^{1/2}_{\omega'}$ in the strong resolvent sense. Now we show that equation (52) does not become uncontrollably large as $\omega$ approaches $\omega'$. To this end we start with an observation that the (non-continuous) function $f$ can be replaced by a continuous one $f_1$.

$$\begin{aligned}\| f(\Delta_{\omega,\omega'})\varrho^{1/2}\| &= \left\| \int_0^1 f(\lambda)\, \mathrm{d}E_{\omega,\omega'}(\lambda)\, \varrho^{1/2} + \int_1^\infty f(\lambda) \mathrm{d}E_{\omega,\omega'}(\lambda)\, \varrho^{1/2} \right\| \\ &= \left\| \int_0^1 f(\lambda)\, \mathrm{d}E_{\omega,\omega'}(\lambda)\, \varrho^{1/2} + \int_1^\infty \mathrm{d}E_{\omega,\omega'}(\lambda)\, \varrho^{1/2} - 2\int_1^\infty \mathrm{d}E_{\omega,\omega'}(\lambda)\, \varrho^{1/2} \right\|.\end{aligned}$$

Denote by $P = \int_1^\infty \mathrm{d}E_{\omega,\omega'}(\lambda)$ ($P$ is a projector). So

$$\begin{aligned}\| f(\Delta_{\omega,\omega'})\varrho^{1/2}\| &\leqslant \left\| \int_0^\infty f_1(\lambda)\, \mathrm{d}E_{\omega,\omega'}(\lambda)\, \varrho^{1/2} \right\| + 2\|P\varrho^{1/2}\| \\ &\leqslant \left\| \int_0^\infty f_1(\lambda)\, \mathrm{d}E_{\omega,\omega'}(\lambda)\, \varrho^{1/2} \right\| + 2\|\varrho^{1/2}\| = \| f_1(\Delta_{\omega,\omega'})\varrho^{1/2}\| + 2\|\varrho^{1/2}\|\end{aligned} \tag{53}$$

where

$$f_1(x) = \begin{cases} 1 & \text{if } x \geqslant 1 \\ x^{-1} & \text{if } 0 < x < 1. \end{cases}$$

Now let $g$ be a bounded continuous function. The strong resolvent convergence $\Delta^{1/2}_{\omega',\omega}$ to $\Delta^{1/2}_{\omega'}$ implies $g(\Delta^{1/2}_{\omega',\omega})\sigma \to g(\Delta^{1/2}_{\omega'})\sigma$ for any Hilbert–Schmidt operator $\sigma \in \mathcal{H}_{\text{H-S}} \equiv \mathcal{H}_\omega$. This result and the property of the relative modular operator $J\Delta_{\omega',\omega}J = \Delta^{-1}_{\omega,\omega'}$ (cf [3]) imply that

$$g(\Delta^{-1/2}_{\omega,\omega'})\sigma \to Jg(\Delta^{1/2}_{\omega'})J\sigma$$

for any $\sigma \in \mathcal{H}_\omega$ and a bounded function $g$. Define

$$f_0(x) = \begin{cases} 1 & \text{if } x \geqslant 1 \\ x & \text{if } 0 < x < 1. \end{cases}$$

Hence $f_0(\Delta^{1/2}_{\omega',\omega})J\varrho^{1/2} \to f_0(\Delta^{1/2}_{\omega'})J\varrho^{1/2}$ and $f_0(\Delta^{-1/2}_{\omega,\omega'})\varrho^{1/2} \to Jf_0(\Delta^{1/2}_{\omega'})J\varrho^{1/2}$. However, $f_0(\Delta^{-1/2}_{\omega,\omega'})\varrho^{1/2} = f_1(\Delta^{1/2}_{\omega,\omega'})\varrho^{1/2}$ where we have used the assumption that $\varrho^{1/2}$ is in the domain of $\Delta^{-1/2}_{\omega,\omega'}$. This result and equation (53) imply that the set $\{\|f(\Delta^{1/2}_{\omega,\omega'})\varrho^{1/2}\|\}$ is bounded. □

In summary we have

*Theorem 15.* Let $\omega \to \omega'$ in $\beta$-norm where the states $\omega$ and $\omega'$ are faithful ones. Moreover, let $K\omega' \geqslant \omega$ and $\varrho^{1/2}$ be in the domain of $\Delta_{\omega,\omega'}$. Then

$$S(\omega, \omega') \to 0. \tag{54}$$

*Proof.* It is sufficient to show that $\varrho^{1/2}$ is in the domain of $\Delta^{-\frac{1}{2}}_{\omega,\omega'}$. Then the theorem follows directly from lemmas 12 and 14. Let $\omega$ and $\omega'$ be two faithful states on $\mathcal{B}(\mathcal{H})$, i.e. $\omega(A) = \operatorname{Tr}\varrho A$, $A \in \mathcal{B}(\mathcal{H})$ and $\omega'(A) = \operatorname{Tr}\varrho' A$, $A \in \mathcal{B}(\mathcal{H})$ where $\varrho$ and $\varrho'$ are invertible density matrices. Let us assume that $\omega \leqslant K\omega'$, i.e. $\omega(A) \leqslant K\omega'(A)$ for any $A \geqslant 0$ and a fixed positive constant $K$. Hence for any $A \geqslant 0$

$$\operatorname{Tr}(\varrho A) \leqslant K \operatorname{Tr}(\varrho' A). \tag{55}$$

So, for any one-dimensional projector $P_f$,

$$\operatorname{Tr}(\varrho P_f) \leqslant K \operatorname{Tr}(\varrho' P_f). \tag{56}$$

Consequently

$$\varrho \leqslant K\varrho'. \tag{57}$$

We wish to show

$$\varrho^{1/2} \in D(\Delta^{-\frac{1}{2}}_{\omega,\omega'}). \tag{58}$$

Let us observe that equation (58) is equivalent to the following condition:

$$\varrho^{1/2}\varrho^{1/2}(\varrho')^{-\frac{1}{2}} \in \mathcal{H}_{\text{H-S}}. \tag{59}$$

Let us consider the condition (59). We observe that

$$\varrho(\varrho')^{-1/2} \in \mathcal{H}_{\text{H-S}} \qquad \text{iff} \quad \operatorname{Tr}((\varrho')^{-1/2})\varrho^2((\varrho')^{-1/2}) < \infty. \tag{60}$$

Take CONS $\{x_i\}$ such that $\varrho x_i = \lambda_i x_i$. Then

$$\sum (x_i, ((\varrho')^{-1/2})\varrho^2((\varrho')^{-1/2})x_i) = \sum_{ij}(((\varrho')^{-1/2})x_i, x_j)(x_j, \varrho^2((\varrho')^{-1/2})x_i) \tag{61}$$

$$= \sum_{ij} \lambda_j^2(((\varrho')^{-1/2})x_i, x_j)(x_j, ((\varrho')^{-1/2})x_i) \tag{62}$$

$$= \sum_j \lambda_j^2(((\varrho')^{-1/2})x_j, ((\varrho')^{-1/2})x_j) = \sum_j \lambda_j^2(x_j, (\varrho')^{-1}x_j). \tag{63}$$

Let us note that the reversibility of $\varrho$ and $\varrho'$ and the inequality $K\varrho' \geqslant \varrho$ imply

$$K\varrho^{-1} \geqslant (\varrho')^{-1}. \tag{64}$$

Therefore

$$\sum_j \lambda_j^2(x_j, (\varrho')^{-1}x_j) \leqslant K\sum_j \lambda_j^2(x_j, (\varrho)^{-1}x_j) \leqslant K\sum_j \lambda_j < \infty. \tag{65}$$

Thus $\mathrm{Tr}((\varrho')^{-1/2})\varrho^2((\varrho')^{-1/2}) < \infty$ so $\varrho((\varrho')^{-1/2}) \in \mathcal{H}_{\text{H-S}}$ which completes the proof of theorem 15. □

*Remarks 16.* (i) Let us emphasize that the condition $\omega \leqslant K\omega'$ *is simply a quantum translation of the notion 'state close to equilibrium'* (see [24, section III]).
(ii) The condition $\omega \leqslant K\omega'$ implies the boundedness of the analytic extension of non-commutative Radon–Nikodym derivative for general von Neumann algebras (cf [9]). This result in our setting leads to boundedness of $\varrho^{1/2}(\varrho')^{-1/2}$ so to the condition (59).
(iii) The condition $\varrho^{1/2} \in D(\Delta_{\omega,\omega'})$ is the sufficient condition for expressing $||\omega'||_{-\beta}$ in terms of relative modular operator. It is worth pointing out that the inequality $\omega \leqslant K\omega'$ can lead to $\varrho^{1/2} \in D(\Delta_{\omega,\omega'})$. Namely, cf [6, theorem 2.3.19]), $\omega \leqslant K\omega'$ implies in our setting $\varrho = (\varrho')^{1/2}T(\varrho')^{1/2}$ where $T$ is a bounded positive operator. As $\varrho'$ is an invertible density operator, we infer that $T$ is an invertible operator. If additionally, $T^{-1}$ is bounded, then $\varrho^{1/2} \in D(\Delta_{\omega,\omega'})$.

The theorem shows that if states converge to equilibrium in $\|\cdot\|_{-\beta}$-norm, then the relative entropy converges to zero. In [24] the converse of this was obtained in the classical case. It was also shown that for a classical system with countable sample space, the given faithful state is the unique state with $\|\cdot\|_\beta = 1$, all other measures having greater norm. A similar simple argument with Lagrange multipliers gives us the following analogous result.

*Lemma 17.* Let $\rho_\beta$ be a faithful density matrix on $\mathcal{B}(\mathcal{H})$, and define for any density matrix $\rho$ the norm

$$\|\rho\|_{-\beta} = \left(\mathrm{Tr}\,\rho_\beta^{-1}\rho^2\right)^{1/2}.$$

Then $\|\rho\|_{-\beta} \geqslant 1$ with equality if and only if $\rho = \rho_\beta$. □

One can expect that the detailed balance condition, together with the spectral property, should be helpful in the study of the asymptotic behaviour of time evolution. Some results along these lines are presented in [21].

## Acknowledgments

This work was supported by the 'Go East' Programme of the EC, under grant number ERBCIPACT 931672 (nonlinear statistical dynamics), in collaboration with the Nicolas Copernicus University, Toruń. WAM acknowledges partial financial support through KBN grant 2PO3B 14409. WAM wishes to thank the University of London for a Fellowship from the Institute of Mathematics and King's College for extraordinary hospitality.

## References

[1] Agarwal G S 1973 Open quantum Markovian systems and the microreversibility *Z. Phys.* **258** 409–22
[2] Araki H 1976 Relative entropy of states of von Neumann algebras I *Publ. RIMS, Kyoto Univ.* **11** 809
[3] Araki H 1977 Relative entropy of states of von Neumann algebras II *Publ. RIMS, Kyoto Univ.* **13** 173
[4] Alicki R 1976 On the detailed balance condition for non-hamiltonian systems *Rep. Math. Phys.* **10** 249

[5] Boyd R K 1977 Macroscopic and Microscopic Restrictions on Chemical Kinetics *Chem. Rev.* **77** 93

[6] Bratteli O and Robinson D W 1979 *Operator Algebras and Quantum Statistical Mechanics I* (Berlin: Springer)

[7] Bratteli O and Robinson D W 1976 Unbounded derivations of von Neumann algebras *Ann. Inst. H Poincaré* A **25** 139–64

[8] Choi M D 1972 Positive linear maps $C^*$-algebras *Can. J. Math.* **24** 520–9

[9] Connes A 1973 Sur le théorème de Radon–Nikodym pour les poids normaux fidèles semi-finis *Bull. Sc. Math. 2 série* **97** 253–8

[10] Evans D E and Hanche-Oleson H 1979 The generators of positive semigroups *J. Funct. Anal.* **32** 207–12

[11] Frigerio A and Gorini V 1984 Markov dilations and quantum detailed balance *Commun. Math. Phys.* **93** 517–32

[12] Frigerio A and Spohn H 1978 Stationary states of quantum dynamical semi-groups and applications *Lectures at Arco Felice*

[13] Foias C and Sz-Nagy B 1967 *Analyse Harmonique des Operateurs de l'espace de Hilbert* (Budapest: Academiai Kiado)

[14] Glauber R J 1963 Time-dependent statistics for the Ising model *J. Math. Phys.* **4** 294

[15] Hasagawa H and Nakagomi T 1980 On the characterisation of the stationary state of a class of dynamical semigroups *J. Stat. Phys.* **23** 639–52

[16] Kadison R V 1952 A generalized Schwarz inequality and algebraic invariants for operator algebras *Ann. Math.* **56** 494–503

[17] Kossakowski A, Frigerio A, Gorini V and Verri M 1977 Quantum detailed balance and KMS condition *Commun. Math. Phys.* **57** 97–110

[18] Spohn H and Lebowitz J L 1978 Irreversible thermodynamics for quantum systems weakly coupled to thermal reservoirs *Adv. Chem. Phys.* **38** 109

[19] Majewski W A 1984 The detailed balance condition in quantum statistical mechanics *J. Math. Phys.* **25** 614

[20] Majewski W A 1984 Dynamical semigroups in the algebraic formulation of statistical mechanics *Fort. Phys.* **32** 89

[21] Majewski W A 1989 Return to equilibrium and stability of dynamics *J. Stat. Phys.* **55** 417

[22] Narnhofer H and Thirring W 1985 From relative entropy to entropy *Fizika* **17** 257

[23] Powers R T and Størmer E 1970 Free states of the canonical anticommutation relations *Commun. Math. Phys.* **16** 1

[24] Streater R F Detailed balance and free energy *Proc. Symp. on Quantum Information Theory and Open Systems, September 6–8, 1993, (RIMS Kokyuroku Series)* ed M Ohya (Kyoto: RIMS) to be published

[25] Streater R F 1995 *Statistical Dynamics* (London: Imperial College Press)

[26] Streater R F 1994 Entropy and KMS norms *Stochastic Analysis and Applications in Physics* ed L Streit (Dordrecht: Kluwer)

[27] Schatten R 1970 *Norm Ideals of Completely Continuous Operators* (Berlin: Springer)

[28] Tolman R C 1938 *Foundations of Statistical Mechanics* (Oxford: Oxford University Press)