On Master Operators with Extremal Entropy Production

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The master operators **B** which cause the entropy production $\mathrm{d}H/\mathrm{d}t = -k^{-1}\,\mathrm{d}S/\mathrm{d}t$ to become extremal for fixed statistical operators W are constructed and discussed. There are *boundaries* of the set $\mathfrak{B}$ of master operators, $\mathfrak{B} = \{\mathbf{B} \mid \Sigma\, B^2{}_{\nu\mu} = b\}$ for which the problem is solvable yielding minimal entropy production, while no solution exists in the set $\mathfrak{B}$ without any constraints. Operators with maximal entropy production must be extremal points of $\mathfrak{B}$.

I. Introduction

If one tries to deduce the phenomenological theory of macroscopic nonequilibrium systems from a quantum theoretical basis one gets involved into several questions. Let us take up two of these questions.

1. Let be $\{A_i\}$ a set of macroobservables [1], [2]. Then *closed* equations of motion for the expectation values $\langle A_i \rangle$ of the form
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A_i\rangle = \Phi_i(\langle A_j\rangle)$$
must be obtained, but this is impossible if demanded for *every* statistical operator W. Hence selection rules for statistical operators must be formulated.
2. The equations $\langle \dot{A}_i\rangle = \Phi_i(\langle A_j\rangle)$ must be irreversible.

These questions can be treated within the master equation approach. Let be $\mathfrak{H}$ the space of the linear operators on the Hilbert space $\mathscr{H}$ which, for mathematical convenience, is assumed to be of finite dimension. By introduction of an inner product $\mathfrak{H}$ then becomes a Hilbert space again. If the macroobservables A_i commute — we shall assume this property in this paper — then we can simply introduce a subspace $\mathfrak{R} \subset \mathfrak{H}$ generated by the common projection operators P_ν of the A_i:
$$A_i = \sum \alpha_i{}^\nu P_\nu, \quad \mathfrak{R} = \{0 \mid 0 = \sum \omega_\nu P_\nu\}.$$
Given any time evolution $U(t)$ of a statistical operator $U \in \mathfrak{H}$ we can obtain a *second* time evolution $W(t) \in \mathfrak{R}$ by projection of $U(t)$ onto $\mathfrak{R}$. Under certain circumstances this $W(t)$ fulfills a master equation $\dot{W} = \mathbf{B}W$. This master equation in general is irreversible. If now an initial W is macroscopically dispersionless and if this property is conserved in time, then the expectation values $\langle A_i\rangle$ determine the statistical operators by means of
$$\langle A_i\rangle \cong \alpha_i{}^\nu,\ \langle A_i{}^2\rangle \cong (\alpha_i{}^\nu)^2,$$
$$\text{implying } W \cong P_\nu/\dim \mathfrak{r}_\nu .$$
Then the closure property $\langle \dot{A}_i\rangle = \Phi_i(\langle A_j\rangle)$ will be fulfilled. Usually one starts from the projection onto local equilibrium, where the local equilibrium ensemble $\tilde{U}$ is obtained by the solution of the variational problem
$$\delta S[U] = 0\,,$$
$$S = -k_\mathrm{B}\,\mathrm{Sp}(U \log U) = -k_\mathrm{B}\, H[U]\,,$$
$$U \in \mathfrak{V}(\alpha_j) = \{U \mid \mathrm{Sp}(U A_j) = \alpha_j \text{ for all } j\}\,.$$
The solution takes the form $\tilde{U} = C\exp(-\sum \lambda_i A_i)$, hence $\tilde{U} \in \mathfrak{R}$. The entropy $S[\tilde{U}]$ just equals the hydrodynamical entropy. Now it must be shown that the local equilibrium form approximately is conserved in time. Of course, both approaches are closely related.

Now, for the case of commuting macroobservables, no linear operator **C**, neither on $\mathfrak{H}$ nor on $\mathfrak{R}$, does exist, which simultaneously makes the entropy production $\mathrm{d}S/\mathrm{d}t = -k_\mathrm{B}\,\mathrm{Sp}((\mathbf{C}\tilde{U})\log \tilde{U})$ zero and gives the expectation values $\langle \dot{A}_i\rangle = \mathrm{Sp}((\mathbf{C}\tilde{U})A_i)$ nonvanishing values, hence no Euler-like equations can be obtained. It is not clear, though near at hand, that $\tilde{U}$ simultaneously yields the minimal entropy *production* on $\mathfrak{V}$. If one looks for the solution of this question, one gets involved into a difficult nonlinear problem. Now in this paper we reverse this problem: Given a statistical operator $W \in \mathfrak{V}$ we look for those master operators **B** with fixed norm which gives the entropy production extremal values. Having solved this problem — if a solution exists — we then get a lower bound for the minimal entropy production $\dot{S}[\hat{W}]$ by

$$\begin{aligned} &- k_{\mathrm{B}} \min_{W \in \mathfrak{V}} \mathrm{Sp}((\mathbf{B}_{\min}[W]\, W) \log W) \\ &\quad \leqq - k_{\mathrm{B}} \min_{W \in \mathfrak{V}} \mathrm{Sp}((\mathbf{B} W) \log W) \\ &\quad = \dot{S}[\hat{W}] . \end{aligned}$$

This of course is a point of merely technical interest. Let us therefore give an application of more physical interest. The transition probabilities occurring in the master equation can be influenced to some extent by interaction with external systems. Now it is very difficult to list all master operators which can be obtained in this way. Hence, for convenience, we assume that *all* master operators are realizable. Therefore, given the solution of our problem, we can investigate the following *control* problem: We look for a time-dependent master operator $\mathbf{B}(t)$ of fixed norm which makes the relaxation time T^{eq} minimal for a given initial nonequilibrium ensemble. $\mathbf{B}(t)$ then can be chosen as a master operator which gives the entropy production the maximal value for given $W(t)$.

Now we must clarify what is meant by "master operator". From the physical meaning of a statistical operator it follows that it must be Hermitian and positive. For our case of commuting macroobservables it turns out that a statistical operator remains Hermitian and positive only if

$$B_{\nu\mu} = \mathrm{Sp}(P_\nu \mathbf{B} P_\mu) \geqq 0 \quad \text{for} \quad \nu \neq \mu$$

and $B_{\mu\mu} \leqq 0$. Furthermore we must demand that $\mathbf{B} W^{\mathrm{eq}} = 0$ and $\mathrm{Sp}(1\, W) = 0$. If the Hilbert space $\mathscr{H}$ is chosen to be an energy shell, these latter conditions imply very simple additional sum rules for the matrix elements $B_{\nu\mu}$: $\sum_\nu B_{\nu\mu} = \sum_\mu B_{\nu\mu} = 0$. Then all operators with these properties are called master operators. The entropy production for a given master operator then is given by

$$\mathrm{d}S/\mathrm{d}t = - k_{\mathrm{B}} \sum B_{\nu\mu} \log w_\nu\, w_\mu$$

with $W = \sum w_\nu P_\nu$. It should be noted that the form of the entropy production and the form of the conditions given above depend on the choice of commuting macroobservables. This choice is near at hand, it follows from the usual philosophy of macroobservables, but on the other hand it excludes the possibility of nontrivial entropy conserving equations as mentioned above.

Now our problem is a linear one, it can be solved by simple geometrical techniques. We introduce a vector space $\mathbb{R}^{\varrho^2}$, where ϱ is the dimension of the space $\mathfrak{R}$ generated by the operators P_ν. Then we consider the elements $B_{\nu\mu}$ and the numbers $\log w_\nu\, w_\mu$ as components of vectors $B, X \in \mathbb{R}^{\varrho^2}$, thus $\mathrm{d}H/\mathrm{d}t = \langle B, X \rangle$. Hence, if a solution of the problem exists, it is obtained by simple projection techniques. The additional question whether solutions do exist or not turns out to be much more difficult. Let be $\mathfrak{B}$ the domain of all master operators with $\sum B_{\nu\mu}^2 = b$, then no solution exists in $\mathring{\mathfrak{B}}$ for any W. On the other hand there are boundary pieces for which a solution exists. Thus the difficult problem arises for which boundary pieces solutions exist. We don't give the general solution of this problem in this paper.

Let us give a short statement of contents. In Sect. II we derive the form of the solution by projection techniques, then we give our first example: No solution exists in $\mathring{\mathfrak{B}}$. After that we give the solution an analytical form by means of a series expansion, using functional analytical methods. In Sect. III we take the first step in solving the general problem mentioned above: We prove the existence of solutions for certain boundary pieces which are part of boundary pieces of higher dimension, whenever the problem is solvable for these latter pieces. In the following Sect. IV we construct a solution and investigate an additional example for insolvability. After that we investigate the entropy production for boundary pieces of dimension 0. Using convexity arguments we get a new proof of the well-known result, that the entropy production always is negative [4].

Thus we get bounds for every $W \neq W^{\mathrm{eq}}$. It would be interesting to investigate if there are any dualities between master operators and statistical operators. This idea originates from the form of the entropy production: It is given by an ordinary inner product, $\mathrm{d}H/\mathrm{d}t = \langle B, X \rangle$. Moreover, any solution takes the form $B_{\nu\mu} = \gamma\, \eta_{\nu\mu}(X_{\nu\mu} + \lambda_\nu + \gamma_\mu)$. where $\eta_{\nu\mu}$ is given by

$$\eta_{\nu\mu} = \left\{ \begin{matrix} 1 & \text{for some pairs } (\nu, \mu) \\ 0 & \text{for the remaining pairs} \end{matrix} \right\},$$

γ is a constant.

II. Construction of the Extremal Operators

Let be $\mathscr{H}$ an energy shell of finite dimension f, $\mathfrak{H}$ the space of the linear operators on $\mathscr{H}$, $\mathfrak{S}$ a subspace of *commuting* operators (macroobservables) and $\mathfrak{R}$ the space which is spanned by the common projection operators P_ν of the $A_i \in \mathfrak{S}$: $A_i = \sum \alpha_i^\nu P_\nu$. $\mathscr{H}$ becomes a Hilbert-space by introduction of the trace product $(A;B) = \mathrm{Sp}(A^+ B)$ [5].

We assume the validity of a master equation for $W = \mathbf{G}_{\mathfrak{R}} U$, $\mathbf{G}_{\mathfrak{R}}$ is the projection operator onto $\mathfrak{R}$, U the statistical operator in $\mathscr{H}$:

$$\dot{W} = \mathbf{B} W . \tag{1}$$

The solutions of this equation must fulfill

$$W(t) \geqq 0; \quad W(t) = W^+(t) . \tag{2}$$

The conditions (2) imply [6]:

$$\begin{aligned} &(P_\nu; \mathbf{B} P_\mu) = B_{\nu\mu} \in \mathbb{R} , \\ &B_{\nu\mu} \geqq 0 \text{ for } \nu \neq \mu, \quad B_{\nu\nu} \leqq 0 . \end{aligned} \tag{3}$$

Furthermore we have from $\sum P_\nu = f W^{\mathrm{eq}}$:

$$\sum_\nu B_{\nu\mu} = \sum_\mu B_{\nu\mu} = 0 . \tag{4}$$

Regarding $B_{\nu\mu}$ as components of a vector B the conditions (3) and (4) define a set $\mathfrak{C}$ of vectors:

$$\mathfrak{C} = \left\{ \begin{array}{c} B \mid B_{\nu\mu} \geqq 0 \text{ for } \nu \neq \mu,\ B_{\nu\nu} \leqq 0, \\ \sum_\nu B_{\nu\mu} = \sum_\mu B_{\nu\mu} = 0 \end{array} \right\} . \tag{5}$$

Now let us define

$$H(W) = \mathrm{Sp}(W \log W) , \tag{6}$$

connected with the usual entropy S by $S = -kH$. After a short calculation we get

$$\mathrm{d}H/\mathrm{d}t = \sum B_{\nu\mu} \log w_\nu w_\mu . \tag{7}$$

Now one can look for those operators W, which make the entropy production $\dot{H}$ extremal. This turns out to be a nonlinear problem. Thus we investigate a related question: Given a *fixed* statistical operator W we look for those master operators $B \in \mathfrak{C}$ with $\sum B_{\nu\mu}^2 = b$ which make the entropy production extremal, this is a *linear* problem. Let be $X_{\nu\mu} = \log w_\nu w_\mu$ the components of a vector X. Then we have:

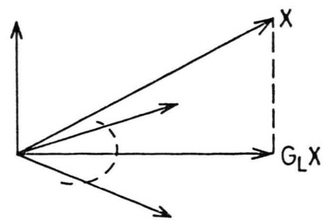
$$\mathrm{d}H/\mathrm{d}t = \langle B, X \rangle . \tag{8}$$

With $B + Z = X$ we get $Z^2 = X^2 + B^2 - 2\langle B, X\rangle$. Thus solutions of our problem are given by those B, which give the distance $\|Z\|$ an extremal value, if $B^2 = \|B\|^2 = b$. Let be L the subspace of $\mathbb{R}^{\varrho^2}$ defined by

$$L = \{Y \mid \sum_\nu Y_{\nu\mu} = \sum_\mu Y_{\nu\mu} = 0\} \tag{9}$$

and let be G_L the projection operator onto L. Then we decompose X: $X = G_L X + (1 - G_L) X$.

Hence extremal distance $\|Z\|$ are obtained for extremal distances $\|G_L X - B\|$:



Now the vectors B fulfill $\|B\|^2 = b$, hence they correspond to points in a sphere of radius $\sqrt{b}$. Therefore, disregarding for the moment the conditions (3), we get two solutions:

$$\begin{aligned} &B_1 = \lambda G_L X, \quad B_2 = -\lambda G_L X , \\ &\lambda^2 = b / \|G_L X\|^2 . \end{aligned}$$

Of course we are not sure that B_1, B_2 fulfill the conditions (3). If this is the case, the entropy production must be negative [4], hence only the negative solution $-\lambda$ is permitted:

$$\begin{aligned} &\mathrm{d}H/\mathrm{d}t = -\lambda \langle G_L X, X \rangle \leqq 0 , \\ &\langle G_L X, X \rangle \geqq 0 . \end{aligned}$$

Hence we have finally: *If* a solution exists, it is given by

$$B = -\frac{\sqrt{b}}{\|G_L X\|} G_L X , \tag{10}$$

the corresponding entropy production is minimal and given by

$$\mathrm{d}H/\mathrm{d}t = -\sqrt{b}\, \|G_L X\| .$$

If there exists no solution we can look for solutions of the problem on the boundary of the set $\mathfrak{B}$:

$$\mathfrak{B} = \mathfrak{C} \cap \{B \mid \|B\|^2 = b\} . \tag{11}$$

The different pieces of the boundary can be characterized by a matrix η: $B \in \partial[\eta]\, \mathfrak{B}$, if

$$B_{\nu\mu} = \eta_{\nu\mu} B_{\nu\mu} , \tag{12}$$

$$\eta_{\nu\mu} = \left\{ \begin{array}{ll} 0, & \text{for } (\nu, \mu) \in M,\ M \text{ a subset} \\ & \text{of the pairs } (\nu, \mu) \\ 1, & \text{else} \end{array} \right\} .$$

Of course $\eta_{\nu\nu} = 0$ implies $\eta_{\nu\mu} = \eta_{\nu\mu} = 0$ with regard to the conditions (4). Then the same method as above applies: Let us regard the space $L[\eta]$, defined by

$$L[\eta] = L \cap \{Y \mid Y_{\nu\mu} = \eta_{\nu\mu} Y_{\nu\mu}\} .$$

Now the question arises, whether there are subspaces $L[\eta]$ for which solutions exist. $G_{L[\eta]}X$ can be calculated by variational techniques, it is the point in $L[\eta]$ with minimal distance from X. We get after a short calculation

$$(G_{L[\eta]}X)_{\nu\mu} = [X_{\nu\mu} + \lambda_\nu + \gamma_\mu]\,\eta_{\nu\mu}\,,$$

where λ_ν, γ_μ are determined by the conditions (4). With $\dim \mathfrak{R} = \varrho$ we get

$$\sum_{\nu=1}^{\varrho}(X_{\nu\mu} + \lambda_\nu + \gamma_\mu)\,\eta_{\nu\mu} = 0\,,$$

$$\sum_{\mu=1}^{\varrho}(X_{\nu\mu} + \lambda_\nu + \gamma_\mu)\,\eta_{\nu\mu} = 0\,. \tag{13}$$

Let us first consider the case $\eta_{\nu\mu} = 1$ for all (ν, μ). Then we get with the abbreviations

$$\begin{aligned}&\sum \lambda_\nu = \lambda, \quad \sum \gamma_\mu = \gamma, \quad \sum \log w_\nu = L\,,\\ &\sum w_\mu = W\colon\ L\,w_\mu + \lambda + \varrho\,\gamma_\mu = 0\,,\\ &\log w_\nu\, W + \varrho\,\lambda_\nu + \gamma = 0 \quad \text{and}\\ &LW + \varrho\,\lambda + \varrho\,\gamma = 0\,.\end{aligned}$$

Hence we get

$$\begin{aligned}\lambda_\nu + \gamma_\mu &= 1/\varrho\,[-\gamma - W\log w_\nu - \lambda - L\,w_\mu]\\ &= -\,W/\varrho\,\log w_\nu - L/\varrho\, w_\mu + LW/\varrho^2,\end{aligned}$$

and

$$\begin{aligned}(G_L X)_{\nu\mu} &= \log w_\nu\, w_\mu - W\log w_\nu/\varrho\\ &\qquad - L/\varrho\, w_\mu + LW/\varrho^2 \quad (14)\\ &= (w_\mu - W/\varrho)\,(\log w_\nu - L/\varrho)\,.\end{aligned}$$

If all w_μ are equal, B vanishes, which violates $\| B \| = \sqrt{b}$. If not all w_μ are equal, then there are positive *and* negative factors among the factors $(w_\mu - W/\varrho)$, $(\log w_\nu - L/\varrho)$. Let be

$$\begin{aligned}w_1 - W/\varrho \quad &\leqq w_2 - W/\varrho \ldots\\ &\leqq w_\varrho - W/\varrho\,,\\ \log w_1 - L/\varrho &\leqq \log w_2 - L/\varrho \ldots\\ &\leqq \log w_\varrho - L/\varrho\,.\end{aligned}$$

We have

$$\begin{aligned}w_1 - W/\varrho < 0\,, \quad \log w_1 - L/\varrho < 0\,,\\ w_\varrho - W/\varrho > 0\,, \quad \log w_\varrho - L/\varrho > 0\,.\end{aligned}$$

Let be $\varrho \geqq 3$. If there is at least one w_σ, $\sigma = 1, \varrho$ with $w_\sigma - W/\varrho < 0$ or $w_\sigma - W/\varrho > 0$, we get a violation of condition (3):

$$\begin{aligned}w_\sigma - W/\varrho < 0 &\Rightarrow (w_\sigma - W/\varrho)(\log w_1 - L/\varrho) > 0\,,\\ w_\sigma - W/\varrho > 0 &\Rightarrow (w_\sigma - W/\varrho)(\log w_\varrho - L/\varrho) > 0\,.\end{aligned}$$

Hence we must have:

$$\sigma \neq 1, \varrho \Rightarrow w_\sigma = W/\varrho, \ \log w_\sigma = L/\varrho\,.$$

Then we get

$$w_1 + w_\varrho + (\varrho - 2)\,W/\varrho = W \Rightarrow W = \varrho/2\,(w_1 + w_\varrho)\,.$$

Analogously we get

$$L = \varrho/2\,(\log w_1 + \log w_\varrho)\,.$$

Now we have

$$\begin{aligned}\log(W/\varrho) = L/\varrho &\Rightarrow \tfrac{1}{2}(\log w_1 + \log w_\varrho)\\ &= \log(\tfrac{1}{2}(w_1 + w_\varrho)) \Rightarrow w_1 = w_\varrho\,.\end{aligned}$$

Hence no solution exists for the case $\varrho \geqq 3$. We get a solution for $\varrho = 2$:

$$G_L X = \begin{bmatrix}(\log w_1 - L/2)(w_1 - W/2), & (\log w_1 - L/2)(w_2 - W/2)\\ (\log w_2 - L/2)(w_1 - W/2), & (\log w_2 - L/2)(w_2 - W/2)\end{bmatrix}. \tag{15}$$

For $\varrho \geqq 3$ there is no solution of the problem. But it is quite possible that there are solutions on the boundaries. Unfortunately there is no simple analytical form of the solution like Eq. (14) for $L[\eta]$. We only can give an expansion of the solution (compare Eqs. (22)—(24)). We define

$$\varrho_\nu = \sum_\mu \eta_{\nu\mu}\,, \quad \sigma_\mu = \sum_\nu \eta_{\nu\mu}$$

and investigate the case ϱ_ν, $\sigma_\mu \neq 0$ for all ν, μ. Let us write

$$\begin{aligned}&\sum_\mu \eta_{\nu\mu}\,A(\mu) = \varrho_\nu\,\{A\}_\nu\,, \quad \sum_\nu \eta_{\nu\mu}\,A(\nu) = \sigma_\mu\,[A]_\mu\,,\\ &\sum_\mu \eta_{\nu\mu}\,X_{\nu\mu} \ = \varrho_\nu\,X_{\nu\{\nu\}}\,, \quad \sum_\nu \eta_{\nu\mu}\,X_{\nu\mu} = \sigma_\mu\,X_{[\mu]\mu}\,.\end{aligned}$$

Thus Eq. (13) reads

$$\begin{aligned}\sigma_\mu(X_{[\mu]\mu} + [\lambda]_\mu + \gamma_\mu) &= 0\,,\\ \varrho_\nu(X_{\nu\{\nu\}} + \lambda_\nu + \{\gamma\}_\nu) \ &= 0\end{aligned}$$

or

$$\begin{aligned}\gamma_\mu &= -\,(X_{[\mu]\mu} + [\lambda]_\mu)\,,\\ \lambda_\nu &= -\,(X_{\nu\{\nu\}} + \{\gamma\}_\nu)\,.\end{aligned} \tag{16}$$

Hence we have

$$\begin{aligned}[\lambda]_\mu &= -\,1/\sigma_\mu \sum_\nu \eta_{\nu\mu}\,X_{\nu[\nu]} - [\{\gamma\}]_\mu\,,\\ \{\gamma\}_\nu &= -\,1/\varrho_\nu \sum_\mu \eta_{\nu\mu}\,X_{[\mu]\mu} - \{[\lambda]\}_\nu\end{aligned}$$

or

$$\gamma_\mu = -X_{[\mu]\mu} + 1/\sigma_\mu \sum_\nu \eta_{\nu\mu} X_{\nu\{\nu\}} + [\{\gamma\}]_\mu ,$$
$$\lambda_\nu = -X_{\nu[\nu]} + 1/\varrho_\nu \sum_\mu \eta_{\nu\mu} X_{\mu[\mu]} + \{[\lambda]\}_\nu . \quad (17)$$

Now let us write

$$\eta_{\nu\mu}/\varrho_\nu = H_{\nu\mu}, \quad \eta_{\varrho\mu}/\sigma_\mu = K_{\varrho\mu},$$
$$-X_{[\mu]\mu} + 1/\sigma_\mu \sum_\nu \eta_{\nu\mu} X_{\nu\{\nu\}} = a_\mu , \quad (18)$$
$$-X_{\nu\{\nu\}} + 1/\varrho_\nu \sum_\mu \eta_{\nu\mu} X_{[\mu]\mu} = b_\nu .$$

Then we get

$$\gamma_\mu = a_\mu + \sum_\varrho K_{\mu\varrho} H_{\varrho\nu} \gamma_\nu , \quad (19\text{a})$$
$$\lambda_\nu = b_\nu + \sum_\varrho H_{\nu\varrho} K_{\varrho\mu} \lambda_\mu . \quad (19\text{b})$$

Of course these equations must be solvable. It turns out that the solutions are not unique, but from our former considerations we know, that $\gamma_\mu + \lambda_\nu$ must be uniquely determined, if $W \neq W^{\text{eq}}$. Let us investigate some properties of the operators $KH = S$, $HK = T$. From the definitions we have the property that $[x]_\mu = 1/\sigma_\mu \sum \eta_{\varrho\mu} X_\varrho$ is an arithmetical mean value, depending on μ, the same is true for $\{x\}_\nu$. Thus we get with $\underline{x} = \min x_\nu$, $\bar{x} = \max x_\nu$: $\underline{x} \leqq [x]_\mu \leqq \bar{x}$, $\underline{x} \leqq \{x\}_\nu \leqq \bar{x}$. Equality only occurs, iff all x_ν are equal. Hence we get

$$\underline{[x]} \leqq \{[x]\}_\nu \leqq \overline{[x]} ,$$
$$\underline{\{x\}} \leqq [\{x\}]_\nu \leqq \overline{\{x\}} .$$

Furthermore we have

$$\underline{x} \leqq \underline{[x]} \leqq \overline{[x]} \leqq \bar{x} ,$$
$$\underline{x} \leqq \underline{\{x\}} \leqq \overline{\{x\}} \leqq \bar{x} .$$

Combining these inequalities we get

$$\underline{x} \leqq \underline{\{[x]\}} \leqq \overline{\{[x]\}} \leqq \bar{x} ,$$
$$\underline{x} \leqq \underline{[\{x\}]} \leqq \overline{[\{x\}]} \leqq \bar{x} ,$$

thus we have with

$$D(\mathfrak{x}) = \bar{x} - \underline{x}: \; D(\mathfrak{x}) \geqq D(T\mathfrak{x}) ,$$
$$D(\mathfrak{x}) \geqq D(S\mathfrak{x}) ,$$

equality only occurs, iff all components of $\mathfrak{x}$ are equal, we then call $\mathfrak{x}$ a *c*-vector. Then we have

$$(\mathbf{1} - T)\mathfrak{x} = 0 \Rightarrow \mathfrak{x} = T\mathfrak{x} \Rightarrow \mathfrak{x} \quad \text{is a c.v.}$$
$$(\mathbf{1} - S)\mathfrak{x} = 0 \qquad \Rightarrow \mathfrak{x} \quad \text{is a c.v.}$$

In the subsequent analysis we denote a c.v. by c. Let us now introduce the operator M:

$$(M\mathfrak{x})_\nu = x_\nu - 1/\varrho \sum x_\mu .$$

If γ is a solution of Eq. (19a), then $M\gamma$ is a solution of the equation:

$$\mathfrak{x} = M\mathfrak{a} + MS\mathfrak{x} .$$

We have:

$$\gamma = \mathfrak{a} + S\gamma \Rightarrow M\gamma = M\mathfrak{a} + MS\gamma ,$$
$$M\gamma = \gamma - c, \quad MSc = 0 \Rightarrow$$
$$M\gamma = M\mathfrak{a} + MS[M\gamma + c]$$
$$= M\mathfrak{a} + MSM\gamma .$$

Analogously we get: If λ is a solution of Eq. (19b), then $M\lambda$ is a solution of the equation

$$\mathfrak{x} = M\mathfrak{b} + MT\mathfrak{x} .$$

But the operators $\mathbf{1} - MT$, $\mathbf{1} - MS$ possess no zero vectors:

$$(\mathbf{1} - MS)\mathfrak{x} = 0 \Rightarrow D(\mathfrak{x}) = D(MS\mathfrak{x}) ,$$
$$D(MS\mathfrak{x}) = D(S\mathfrak{x}) \Rightarrow \mathfrak{x} \text{ is a c.v.} \Rightarrow$$
$$MS\mathfrak{x} = 0 \Rightarrow \mathfrak{x} = 0 .$$

Hence we obtain solutions of Eq. (19a), (19b) by the uniquely determined solutions of the following equations:

$$\gamma = M\mathfrak{a} + MS\gamma , \quad (20\text{a})$$
$$\lambda = M\mathfrak{b} + MT\lambda , \quad (20\text{b})$$

or

$$\gamma = (\mathbf{1} - MS)^{-1} M\mathfrak{a}, \quad \lambda = (\mathbf{1} - MT)^{-1} M\mathfrak{b} .$$

Now let us show that

$$(\mathbf{1} - MS)^{-1} M\mathfrak{a} = \sum_{\nu=0}^{\infty} (MS)^\nu M\mathfrak{a} ,$$
$$(\mathbf{1} - MT)^{-1} M\mathfrak{b} = \sum_{\nu=0}^{\infty} (MT)^\nu M\mathfrak{b} .$$

We have introduced the operators MT, MS, because $\|T\| < 1$, $\|S\| < 1$ is *not* true, we have $Tc = c$, $Sc = c$. It is easily seen that

$$\gamma = \sum_{\nu=0}^{N} (MS)^\nu M\mathfrak{a} + (MS)^{N+1}\gamma .$$

If now $\lim_{N\to\infty} \|(MS)^{N+1}\gamma\| = 0$, then we have obtained the proof without the property $\|MS\| < 1$. We have

$$D(MSM\mathfrak{x}) \leqq D(M\mathfrak{x}) = D\mathfrak{x} .$$

Hence $(d_n) = D((MS)^n M\mathfrak{x})$ decreases monotonously. We show that $\lim d_n = 0$. If $\lim d_n = d > 0$, then we define

$$\mathfrak{M} = \{Y \mid D(Y) = d, \quad g_1 \leqq Y_i \leqq g_2\} .$$

Then there is $(Y_n) \mid Y_n \in \mathfrak{M}$ with

$$\lim \| (MS)^n M \mathfrak{x} - Y_n \| = 0 .$$

$\mathfrak{M}$ is bounded and compact, MS, D are continuous mappings. Hence D takes its upper bound d' on $MS[\mathfrak{M}]$. Now we have $d' < d$: If $d' = d$, then there is $Y^* \in \mathfrak{M}$ with $MSY^* \in \mathfrak{M}$, but then is Y^* a c.v., hence $d = 0$. Therefore we have: $D(MSY_n) \leqq d' < d$. Now D is continuous, therefore we cannot have

$$\lim D((MS)^n M \mathfrak{x}) = d ,$$

hence $\lim d_n = 0$. Then all elements $\in \mathfrak{M}$ are c.v. For all $\varepsilon > 0$ there exists a $n(\varepsilon)$ with

$$m > n(\varepsilon) \Rightarrow \| (MS)^m M \mathfrak{x} - Y_m \| < \varepsilon .$$

Thus we have with $(MS)^n M \mathfrak{x} - Y_n = X_n$:

$$\| X_n \| \to 0 .$$

M is continuous, hence $\| M X_n \| \to 0$. Now

$$M Y_n = 0 \Rightarrow \| (MS)^n M \mathfrak{x} \| \to 0$$

for *all* bounded $\mathfrak{x}$. This is the proof. Therefore we finally have

$$\gamma = \sum_{n=0}^{\infty} (MS)^n M \mathfrak{a} ,$$
$$\lambda = \sum_{n=0}^{\infty} (MT)^n M \mathfrak{b} + c . \tag{21}$$

From Eq. (16) we get $\lambda_\nu = -[X_{\nu\{\nu\}} + \{\gamma\}_\nu]$, hence

$$\sum_{n=0}^{\infty} [(MT)^n]_{\nu\varkappa} b_\varkappa + c_\nu = - X_{\nu\{\nu\}} - \sum_{n=0}^{\infty} H_{\nu\varkappa} [(MS)^n M]_{\varkappa\varrho} a_\varrho ,$$

$$c_\nu = - X_{\nu\{\nu\}} - \sum_{n=0}^{\infty} [(MT)^n M]_{\nu\varkappa} b_\varkappa - \sum_{n=0}^{\infty} H_{\nu\varkappa} [(MS)^n M]_{\varkappa\varrho} a_\varrho = \text{const} = c .$$

The value of c can be obtained by summation:

$$\varrho c = - \sum_\nu X_{\nu\{\nu\}} - \sum_{\nu,\varkappa} \sum_{n=0}^{\infty} [(MT)^n M]_{\nu\varkappa} b_\varkappa - \sum_{\nu,\varkappa,\varrho} \sum_{n=0}^{\infty} H_{\nu\varkappa} [(MS)^n M]_{\varkappa\varrho} a_\varrho .$$

Then we have several different forms of the solution

$$[G_{L[\eta]} X]_{\nu\mu} = [X_{\nu\mu} - X_{\nu\{\nu\}} + \sum_{n=0}^{\infty} \sum_\varkappa (MS)^n{}_{\mu\varkappa} a_\varkappa - \sum_{\varkappa,\lambda} \sum_{n=0}^{\infty} [(MS)^n M]_{\varkappa\lambda} H_{\nu\varkappa} a_\lambda] \, \eta_{\nu\mu} , \tag{22}$$

$$[G_{L[\eta]} X]_{\nu\mu} = [X_{\nu\mu} - X_{[\mu]\mu} + \sum_{n=0}^{\infty} \sum_\varkappa [(MT)^n M]_{\nu\varkappa} b_\varkappa - \sum_{n=0}^{\infty} \sum_{\varkappa,\lambda} K_{\mu\varkappa} [(MT)^n M]_{\varkappa\lambda} b_\lambda] \, \eta_{\nu\mu} , \tag{23}$$

$$[G_{L[\eta]} X]_{\nu\mu} = [X_{\nu\mu} + \sum_{n=0}^{\infty} \sum_\varkappa [(MT)^n M]_{\nu\varkappa} b_\varkappa + \sum_{n=0}^{\infty} \sum_\varkappa [(MS)^n M]_{\mu\varkappa} a_\varkappa + c] \, \eta_{\nu\mu} . \tag{24}$$

a_μ, $b_\varkappa$ are defined in Eqs. (17). Note that these equations are valid for *any* vector $(X_{\nu\mu})$.

Now, however, the question still remains open under which circumstances the solutions fulfill our conditions (3). There are several possibilities:

1) The investigation of additional examples,
2) General investigations of the solutions (22)—(24),
3) General topological investigations,
4) The sign of the entropy production.

The first possibility — compare our first example for insolvability — at first glance yields the conjecture, that no solution $B \in [\partial[\eta] \mathfrak{B}]^0$ exists for any η. The proof of this conjecture is difficult, because the general form of the solution is too complicated. The possibility 4) depends on the fact that $\mathrm{d}H/\mathrm{d}t \leqq 0$ for every master operator and for every W. Now, if B is a master operator, we must have

$$- \sqrt{b} / \| G_{L[\eta]} X \| \, \langle G_{L[\eta]} X[W_1], Y[W_2] \rangle \leqq 0 ,$$

hence $\langle G_{L[\eta]} X[W_1], Y[W_2] \rangle \geqq 0$.

The third possibility investigates the existence of solutions $G_{L[\eta]} X$, if a solution $G_{L[\tilde{\eta}]} X$ exists with $L[\eta] \subset L[\tilde{\eta}]$.

Let us first prove a theorem. This theorem reduces the general problem of solvability to a special one: If no solution exists for a special class of matrices, then no solution does exist in the general case. Now we can construct a solution for a matrix which belongs to the special class mentioned above. Therefore the conjecture is not true.

III. Proof of a Theorem

Theorem. (25)

Let be $L[\eta]$ a space of dimension $k \geqq 3$. If $G_{L[\eta]} X$ is a negative master operator with

$$G_{L[\eta]} X \in [\partial[\eta] \mathfrak{B}]^0 ,$$

then there exists a subspace

$$L[\tilde{\eta}] \subset L[\eta], \quad 2 \leqq \dim L[\tilde{\eta}] < k$$

with the property that $G_{L[\tilde{\eta}]}X$ is a negative master operator again and $G_{L[\tilde{\eta}]}X \in [\partial[\tilde{\eta}]\,\mathfrak{B}]^0$.

Proof. Let us define

$$\mathscr{C}[\eta, A] = \left\{ \begin{matrix} X \,|\, \sum_\nu X_{\nu\mu} = \sum_\mu X_{\nu\mu} = 0, \; X_{\nu\nu} \geqq 0, \; X_{\nu\mu} \leqq 0, \\ X_{\nu\mu} = \eta_{\nu\mu} X_{\nu\mu}, \quad |X_{\nu\mu}| \leqq A \end{matrix} \right\}, \tag{26}$$

where A is an arbitrary constant. Then $\mathscr{C}[\eta, A]$ is a convex polyhedron, which can be generated by its extremal points X_l:

$$X \in \mathscr{C}[\eta, A] \Rightarrow X = \sum \lambda_l X_l \,|\, \lambda_l \geqq 0, \; \sum \lambda_l = 1.$$

Now $G_{L[\eta]}X \in [\mathscr{C}[\eta, A]]^0$. Let be Y a point $\in \partial\mathscr{C}[\eta, A]$ with minimal distance:

$$Y' \in \partial\mathscr{C}[\eta, A] \Rightarrow \| Y' - G_{L[\eta]}X \| \geqq \| Y - G_{L[\eta]}X \| .$$

Now we have $Y \in L[\tilde{\eta}]$. If this is not the case, we can enlarge the constant A. Now Y cannot take the form $Y = \alpha X_k$, (note that 0 is an extremal point). If this were the case we would have

$$\| G_{L[\eta]}X - \alpha X_k \| \leqq \| G_{L[\eta]}X - \alpha X_k - \beta X_l \| ,$$

at least for sufficiently small positive β. We have

$$\alpha X_k + \beta X_l \in \partial\mathscr{C}[\eta, A] .$$

Then we get after a short calculation:

$$2 \langle X_l, G_{L[\eta]}X - \alpha X_k \rangle \leqq \beta \| X_l \|^2 \Rightarrow \langle X_l, G_{L[\eta]}X - \alpha X_k \rangle \leqq 0 .$$

Now we have, with G_k being the projection operator onto the space (X_k):

$$\alpha X_k = G_k G_{L[\eta]} X ,$$

thus

$$\alpha = \langle X_k, G_{L[\eta]} X \rangle / \| X_k \|^2$$

and therefore

$$\langle X_l, G_{L[\eta]} X \rangle \leqq \langle X_l, X_k \rangle \langle X_k, G_{L[\eta]} X \rangle / \| X_k \|^2$$

for *all* l. Now $G_{L[\eta]}X = \sum \lambda_j X_j$, hence

$$\sum_l \lambda_l \langle X_l, \sum \lambda_j X_j \rangle \leqq \sum_l \lambda_l \langle X_l, X_k \rangle \langle X_k | \sum \lambda_j X_j \rangle / \| X_k \|^2 ,$$

$$\| G_{L[\eta]} X \|^2 \leqq \langle G_{L[\eta]} X, X_k \rangle \langle X_k, G_{L[\eta]} X \rangle / \| X_k \|^2 ,$$

which implies $G_{L[\eta]}X \parallel X_k$. This contradicts

$$G_{L[\eta]} X \in [\partial[\eta]\,\mathfrak{B}^0 .$$

Thus we have $Y = \sum \alpha_i X_i$, $\alpha_i \geqq 0$, where at least two $\alpha_i \neq 0$.

Hence we have

$$Y = \sum_{i \in R} \alpha_i X_i , \quad i \in R \Rightarrow \alpha_i > 0 .$$

Then we have

$$Y \in H(X_i, i \in R) , \quad H(X_i, i \in R) = L[\tilde{\eta}] .$$

Now we get $L[\tilde{\eta}] \subset L[\eta]$, hence

$$G_{L[\tilde{\eta}]} G_{L[\eta]} X = G_{L[\tilde{\eta}]} X = Y .$$

Of course these considerations can be repeated with the space $L[\tilde{\eta}]$. Therefore we have the following result: If there is an inner solution $G_{L[\eta]}X$, then there must be a space $L[\tilde{\eta}]$ of dimension 2 with $G_{L[\tilde{\eta}]}X \in [\partial[\tilde{\eta}]\,\mathfrak{B}]^0$.

Hence the conjecture from Sect. II can be checked by investigation of all matrices η which yield a space $L[\eta]$ of dimension 2. If *no* matrix η of this kind does exist with $G_{L[\eta]}X \in [\partial[\eta]\,\mathfrak{B}]^0$, then *no* inner solution can exist at all. If on the other hand a matrix η of the kind considered yield a solution, then, of course, one cannot conversely conclude that inner solutions in spaces $L[\eta']$ of higher dimensions do exist.

IV. Construction of an Inner Solution

Let us consider a special extremal matrix η_1. This matrix has nonvanishing diagonal elements and in any row and in any column there are exactly two nonvanishing elements. For example: $\varrho = 4$,

$$\eta_1 = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \end{pmatrix}.$$

The corresponding operator X_1 is given by ($X_1 \triangleq B$)

$$B_{\nu\mu} = 1/\sqrt{2\varrho}\,(\delta_{\nu\mu} - \delta_{\mu\mu(\nu)}) , \tag{27}$$

where $\mu(\nu)$ determines the nonvanishing off-diagonal element in the row ν. For convenience we have chosen $\sum B_{\nu\mu}^2 = 1$. Now let us regard a matrix η' with $\eta'_{\nu\mu} = \eta^1_{\nu\mu} + \delta_{\nu i}\delta_{\mu j}$. Then we construct a third matrix η_2

$$\eta^2_{\nu\mu} = \begin{Bmatrix} \eta^1_{\nu\mu} + \delta_{\nu i}\,\delta_{\mu j}\,, & \text{for } \nu \neq \mu(i),\, \mu \neq \mu(i) \\ 0 & ,\ \text{else} \end{Bmatrix}. \quad (28)$$

Furthermore we presuppose that $\mu(\mu(i)) = j$, the reason will become clear at one. For example: $\varrho = 4$,

$$\eta' = \begin{pmatrix} 1 & 1 & [1] & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \eta^2 = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

η^2 now has just two elements in any row and in any column. Only the row $\mu(i)$ and the column $\mu(i)$ contain only vanishing elements. η^2 thus is an extremal matrix and the corresponding operator X_2 is constructed in the same manner as above.

Now let us consider the space generated by the normed vectors X_1, X_2, which correspond to our operators. We have

$$\alpha X_1 + \beta X_2 \in L[\eta'] .$$

If $\alpha, \beta > 0$, then the corresponding operator is a negative master operator. Clearly we have:

$$\dim L[\eta'] = 2 .$$

Now let us consider $G_{L(\eta')}\, X$:

$$G_{L[\eta']}\, X = \alpha X_1 + \beta X_2 \Rightarrow$$
$$\alpha + \beta \langle X_1, X_2 \rangle = \langle X_1, X \rangle ,$$
$$\alpha \langle X_1, X_2 \rangle + \beta = \langle X_2, X \rangle .$$

Let us abbreviate: $\varphi = \langle X_1, X_2 \rangle$, $\dot{H}_1 = \langle X_1, X \rangle$, $\dot{H}_2 = \langle X_2, X \rangle$. Then the solution of the latter equation is

$$\alpha = \frac{1}{1-\varphi^2} (\dot{H}_1 - \varphi \dot{H}_2) ,$$
$$\beta = \frac{1}{1-\varphi^2} (-\varphi \dot{H}_1 + \dot{H}_2) . \quad (29)$$

Now φ, $\dot{H}_1$, $\dot{H}_2$ are positive numbers (compare Eqs. (8), (10)). φ is given by

$$\varphi = \frac{2\varrho - 3}{2\varrho} \sqrt{\frac{\varrho}{\varrho - 1}} .$$

Hence

$$\dot{H}_1 = \sum \log w_\nu w_\nu \sqrt{\frac{1}{2\varrho}} - \sum_{\nu \neq \mu} \log w_\nu w_\mu \eta_{\nu\mu} \sqrt{\frac{1}{2\varrho}} , \quad (30)$$

$$\dot{H}_2 = \sum_{\nu \neq \mu(i)} \log w_\nu w_\nu \sqrt{\frac{1}{2\varrho - 2}} - \sum_{\nu \neq \mu} \log w_\nu w_\mu \eta_{\nu\mu}[X_2] \sqrt{\frac{1}{2\varrho - 2}} . \quad (31)$$

Thus we get:

$$\sqrt{2\varrho - 2}\, \dot{H}_2 = \sum \log w_\nu w_\nu - \log w_{\mu(i)} w_{\mu(i)} - \log w_i w_j + \log w_i w_{\mu(i)} + \log w_{\mu(i)} w_j - \sum_{\nu \neq \mu} \log w_\nu w_\mu \eta_{\nu\mu}[X_1] .$$

For abbreviation:

$$[\log w_i - \log w_{\mu(i)}][w_{\mu(i)} - w_j] = y . \quad (32)$$

Then we get

$$\sqrt{2\varrho - 2}\, \dot{H}_2 = \sqrt{2\varrho}\, \dot{H}_1 + y , \quad (33)$$

and hence

$$\dot{H}_1 - \varphi \dot{H}_2 = \dot{H}_1 / 2\varrho - 2 , \quad (34)$$
$$H_1/2\varrho - 2 - 2(\varrho - 3) - (2\varrho - 3) \sqrt{2\varrho}/4\varrho(\varrho - 1) \cdot y ,$$
$$\dot{H}_2 - \varphi \dot{H}_1 = 3\dot{H}_2/2\varrho + \frac{(2\varrho - 3)\, y}{2\sqrt{2\varrho}\sqrt{\varrho - 1}} .$$

These expressions must be positive in order to get a solution. But this is possible, if $y = 0$.

Now:

$$y = 0 \Rightarrow w_{\mu(i)} = w_j \quad \text{or} \quad \log w_i = \log w_{\mu(i)} .$$

Hence a solution is obtained, if $\dot{H}_1, \dot{H}_2 > 0$. One is able to fulfill this condition for the example given above. We get:

$$\varrho = 4, \quad \varphi = \sqrt{25/48} ,$$
$$\dot{H}_1 = (1/\sqrt{8}) [\log w - \log w_4][w - w_4] ,$$
$$\dot{H}_2 = (1/\sqrt{6}) [\log w - \log w_4][w - w_4] ,$$

where, for convenience, $w = w_1 = w_2 = w_3$, $w_4 \neq w$. For reasons of continuity the solvability conditions remain fulfilled for sufficiently small $|y|$. With

$$\dot{H}_2 = \sqrt{1/2\varrho - 2}\, \dot{S}_2, \quad \dot{H}_1 = \sqrt{1/2\varrho}\, \dot{S}_1$$

we obtain $\dot{S}_2 = \dot{S}_1 + y$. Hence

$$\dot{H}_1 - \varphi \dot{H}_2 = \sqrt{1/2\varrho}\, 1/(2\varrho - 2) [\dot{S}_1 - 2\varrho y + 3y] ,$$
$$\dot{H}_2 - \varphi \dot{H}_1 = \sqrt{1/2\varrho - 2}\, 1/2\varrho [3\dot{S}_2 + 2\varrho y - 3y]$$

or

$$\dot{H}_1 - \varphi \dot{H}_2 = \sqrt{1/2\varrho}\, 1/(2\varrho - 2) [3\dot{S}_2 - (2\varrho y + 2\dot{S}_1)],$$
$$\dot{H}_2 - \varphi \dot{H}_1 = \sqrt{1/2\varrho - 2}\, 1/2\varrho [3\dot{S}_1 + 2\varrho y]$$

or

$$\dot{H}_1 - \varphi\,\dot{H}_2 = \sqrt{1/2\,\varrho}\,1/(2\,\varrho - 2)\,[\dot{S}_1 - (2\,\varrho - 3)\,y]\,,$$
$$\dot{H}_2 - \varphi\,\dot{H}_1 = \sqrt{1/2\,\varrho - 2}\,1/2\,\varrho\,[\dot{S}_1 + 2/3\,\varrho\,y]\,. \qquad (35)$$

Hence all $X[W]$ with

$$\dot{S}_1 > (2\,\varrho - 3)\,y \quad \text{and} \quad \dot{S}_1 > -\,2/3\,\varrho\,y$$

yield a $G_{L(\eta')}X$ which is a negative master operator.

Let us now investigate the case $\varrho = 3$. Then the conditions read: $\dot{S}_1 > 3y$, $\dot{S}_1 > -y/2$. With

$$\eta_1 = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}, \quad \eta_2 = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix},$$

$$\eta' = \begin{pmatrix} 1 & 1 & [1] \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}, \quad i = 1,\; j = 3,\; \mu(i) = 2\,,$$

we have

$$y \;= [\log w_1 - \log w_2]\,[w_2 - w_3]\,,$$
$$\dot{S}_1 = \log w_1 (w_1 - w_2) + \log w_2 (w_2 - w_3) + \log w_3 (w_3 - w_1)\,.$$

If $y > 0$, then the ocndition reads $\dot{S}_1 > 3y$,

$$y < 0 \;\Rightarrow\; S_1 > |y|/2\,.$$

We don't answer the question whether there is a W which fulfills this condition or not.

Instead of that let us give an example which shows that there are matrices η for which no solution exists. We consider a matrix η with $\eta_{\nu\mu} = 1$, only $\eta_{ij} = 0$, $i \neq j$. We get after a lengthy calculation with $G_{L(\eta)}X = B$:

$$B_{\nu\mu} = (w_\mu - W)(\log w_\nu - L) - (1/\varrho - 1)^2 (w_j - W)(\log w_i - L) \quad \text{for} \quad \nu \neq i,\; \mu \neq j\,, \qquad (36\text{a})$$

$$B_{ij} \;= 0\,, \qquad (36\text{b})$$

$$B_{i\mu} = (\log w_i - L)\,[(w_\mu - W) + (w_j - W)/\varrho - 1], \quad \mu \neq j, \qquad (36\text{c})$$

$$B_{\nu j} \;= (w_j - W)\,[(\log w_\nu - L) + (\log w_i - L)/\varrho - 1], \quad \nu \neq i\,, \qquad (36\text{d})$$

with $W = \sum w_\mu/\varrho$, $L = \sum \log w_\mu/\varrho$ (compare Eq. (13)). Let us choose $w_1 \leqq w_2 \leqq \cdots \leqq w_\varrho$. This can be obtained by permutation of the indices, the new pair $(i'\,j')$ again can be denoted by (i, j). If all w_μ are equal, then we have $B = 0$. Now, if all w_μ with $\mu \neq i, j$ are equal, then from Eq. (36a) it follows that all $B_{\nu\mu}$ with ν, $\mu \neq i, j$ are equal. Now:

$$B_{\nu\mu} \leqq 0 \leqq B_{\nu\nu} \;\Rightarrow\; B_{\nu\mu} = B_{\nu\nu} = 0\,.$$

Hence all $B_{\nu\mu} = 0$ for ν, $\mu \neq i, j$, if $\varrho > 3$. But then $B_{i\mu} = B_{\nu j} = 0$, which implies with $B_{ij} = 0$:

$$B_{ii} = 0, \quad B_{ji} = 0 \quad \text{or} \quad B = 0\,.$$

Let us now investigate the case $\varrho > 3$ and let us first assume that $(w_j - W)(\log w_i - L) \neq 0$. From Eq. (36a) it follows that

$$\begin{Bmatrix} (w_\mu - W)(\log w_\nu - L) \\ (w_\nu - W)(\log w_\mu - L) \end{Bmatrix} \leqq \begin{Bmatrix} (w_\mu - W)(\log w_\mu - L) \\ (w_\nu - W)(\log w_\nu - L) \end{Bmatrix}.$$

Any equality then implies

$$B_{\nu\mu} = B_{\nu\nu} = B_{\mu\nu} = B_{\mu\mu} = 0\,.$$

Let be, for instance,

$$(w_\mu - W)(\log w_\nu - L) = (w_\mu - W)(\log w_\mu - L)\,.$$

Then we have $B_{\nu\mu} = B_{\mu\mu} = 0$. Now

$$(w_\mu - W)(\log w_\nu - L) \neq 0 \;\Rightarrow\; \log w_\nu = \log w_\mu \;\Rightarrow\; w_\nu = w_\mu \;\Rightarrow\; B_{\nu\nu} = B_{\mu\nu} = 0\,.$$

Hence we get

$$(w_j - W)(\log w_i - L) \neq 0\,, \quad w_\mu < w_\nu \;\Rightarrow\; w_\mu < W, \quad \log w_\nu > L, \quad w_\nu > W, \quad \log w_\mu < L\,,$$

and

$$(w_j - W)(\log w_i - L) \neq 0, \quad w_\nu < w_\mu \;\Rightarrow\; w_\mu > W, \quad \log w_\nu < L, \quad w_\nu < W, \quad \log w_\mu > L$$

or

$$w_\mu < w_\nu \;\Rightarrow\; w_\mu < W < w_\nu, \quad \log w_\mu < L < \log w_\nu\,.$$

Analogously we get

$$w_\mu > w_\nu \;\Rightarrow\; w_\nu < W < w_\mu\,, \quad \log w_\nu < L < \log w_\mu\,.$$

Thus we have

$$w_\mu < w_\nu \leqq W \;\Rightarrow\; w_\mu \geqq w_\nu\,,$$

or

$$w_\mu, w_\nu \;\; \leqq W \;\Rightarrow\; w_\mu = w_\nu\,,$$
$$w_\mu, w_\nu \;\; \geqq W \;\Rightarrow\; w_\mu = w_\nu\,.$$

Then we get

$$[B_{\mu\mu} > 0 \;\Rightarrow\; w_\mu \neq w_\nu \text{ for all } \nu \neq i, j] \;\Rightarrow$$
$$[w_\mu \leqq W \;\Rightarrow\; w_\nu > W]\,,$$
$$(w_\mu \geqq W \;\Rightarrow\; w_\nu < W]\,.$$

But then we have

$$B_{\nu\nu} = 0, \quad B_{\nu\mu} = B_{\mu\nu} = 0 \Rightarrow$$
$$w_\mu = w_\nu \Rightarrow B_{\mu\mu} = 0 .$$

Thus $B = 0$.

Therefore we must have $(w_j - W)(\log w_i - L) = 0$. Let be $w_j = W$, $\log w_i \neq L$. Then Eq. (36d) implies

$$B_{\nu j} = 0, \quad B_{ij} = 0 \Rightarrow B_{ii} = 0 \Rightarrow B_{i\mu} = 0.$$

Hence from Eq. (36c) we have $w_\mu = W$ for $\mu \neq j$. Hence all w_ν are equal $\Rightarrow B = 0$. The same is true for $\log w_i = L$, $w_j \neq W$. Thus we are left with $w_j = W$, $\log w_i = L$. Therefore we get

$$B_{\nu\mu} = (w_\mu - W)(\log w_\nu - L)$$

for *all* ν, μ including i, j and $w_j = W$, $\log w_i = L$. But this implies

$$B = 0 \tag{37}$$

as shown in Section II. Hence we have obtained a second example for non-solvability.

V. Entropy Production on Boundaries of Dimension 1

The result obtained up to now is that the entropy production possesses analytical extremal values inside certain boundary pieces. These values are minimal values. On the other hand the entropy production $\mathrm{d}H/\mathrm{d}t$ (8) is a continuous function on the set $\mathfrak{B}$ (11). $\mathfrak{B}$ is compact and bounded, hence $\mathrm{d}H/\mathrm{d}t$ must take its extremal values in $\mathfrak{B}$. The maximal value must be obtained for an extremal master operator, because no analytical maximum exists. We have from $\mathrm{d}H/\mathrm{d}t = \sum \log w_\nu w_\mu B_{\nu\mu}$ if B is an extremal operator:

$$\mathrm{d}H/\mathrm{d}t = -\sqrt{b/2\sigma} \sum \log w_\nu (w_\nu - w_{s(\nu)}) \tag{38}$$

with $\sigma = \sum \eta_{\nu\nu}$. In every row ν there is just one non-vanishing $\eta_{\nu s(\nu)}$, in every column μ we have just one non-vanishing $\eta_{z(\mu)\mu}$. Now let us show that $\mathrm{d}H/\mathrm{d}t \leqq 0$. Of course, this result has been used previously. We regard the variational problem $\delta(\mathrm{d}H/\mathrm{d}t) = 0$ now for a *fixed* extremal master operator under the constraints $\sum s_\nu w_\nu = 1$, $w_\nu \geqq 0$. This problem is less difficult than the general one. We get

$$\mathrm{d}H/\mathrm{d}t = -\sqrt{b/2\sigma}\,[\sum w_\mu \log w_\mu \eta_{\mu\mu} - \sum (\eta_{\nu\mu} - \delta_{\nu\mu}) w_\mu \log w_\nu] .$$

Hence

$$\begin{aligned} \mathrm{d}/\mathrm{d}\varepsilon \{ -\sqrt{b/2\sigma}\,[2 \sum (\bar{w}_\mu + \varepsilon u_\mu)(\log(\bar{w}_\mu + \varepsilon u_\mu)) \\ - \sum \eta_{\nu\mu} (\bar{w}_\mu + \varepsilon u_\mu)(\log(\bar{w}_\nu + \varepsilon u_\nu)) \\ + \lambda \sum s_\nu (\bar{w}_\nu + \varepsilon u_\nu)] \} = 0 \quad \text{for} \quad \varepsilon = 0 \end{aligned}$$

where u_μ is a test vector. If all $\bar{w}_\nu > 0$, then we get with $u_\mu = \delta_{\mu\varkappa}$

$$\begin{aligned} 2[\log \bar{w}_\varkappa + 1] - \sum \eta_{\nu\varkappa} \log \bar{w}_\nu \\ - \sum \eta_{\varkappa\mu} \bar{w}_\mu / \bar{w}_\varkappa + \lambda s_\varkappa = 0 \\ \Rightarrow \bar{w}_\varkappa \log \bar{w}_\varkappa + \bar{w}_\varkappa - \bar{w}_\varkappa \log \bar{w}_{z(\varkappa)} - \bar{w}_{s(\varkappa)} \\ = -\lambda s_\varkappa \bar{w}_\varkappa , \end{aligned} \tag{39}$$

where we have used that

$$\begin{aligned} \mathrm{d}H/\mathrm{d}t &= -\sqrt{b/2\sigma} \sum \log w_\nu (w_\nu - w_{s(\nu)}) \\ &= -\sqrt{b/2\sigma} \sum \log w_\nu (w_\nu - w_{z(\nu)}) . \end{aligned} \tag{40}$$

If $\lambda > 0$, we regard $\bar{w}_\varkappa = \bar{w} = \sup w_\nu$ which yields a contradiction, analogously $\lambda < 0$ yields a contradiction with $\bar{w}_\varkappa = \underline{w} = \inf w_\nu$. For $\lambda = 0$ all $\bar{w}_\nu$ are equal. Hence we get:

$$\bar{w}_\nu > 0 \quad \text{for all} \quad \nu \Rightarrow \bar{w}_\nu = \text{const.}$$

Now let us consider the case that some of the w_ν are zero a priori. If we don't have

$$\begin{aligned} w_\alpha = 0 \Rightarrow w_{s(\alpha)} = 0 \\ (\Rightarrow (w_{z(\beta)} = 0 \Rightarrow w_\beta = 0)) , \end{aligned} \tag{41}$$

then we get $\mathrm{d}H/\mathrm{d}t = -\infty$. In this case we must have in mind that in the derivation of the master equation there appears a time τ corresponding to a difference equation, so this divergence is an artificial one due to our use of the differential calculus. Let us now consider only those W for which the condition (41) is fulfilled. Then all terms in Eqs. (39) remain bounded, if only those w_ν are taken into account which are not zero a priori. Then the same argument as above shows that the only solutions are given by $\bar{w}_\nu = \text{const}$, $\bar{w}_\mu = 0$ corresponding to $\lambda = 0$. A simple calculation then yields, that all correspond to maxima of the entropy production $\mathrm{d}H/\mathrm{d}t$, $\mathrm{d}H/\mathrm{d}t = 0$. Thus all *minima* — if existing — must be given by extremal points of the convex polyhedron

$$\mathbb{T} = \{ W \mid w_\nu \geqq 0 \wedge \sum s_\nu w_\nu = 1 \} .$$

These extremal points are given by

$$W_{\mathrm{ex}} = \{ w_\nu \mid w_\nu = \delta_{\nu\varkappa} / s_\varkappa \} .$$

They do not fulfill the condition (41). Hence we get the result: $\mathrm{d}H/\mathrm{d}t$ possesses maxima in every boundary piece of $\mathbb{T}$ if only those W are regarded which fulfill the conditions (41) — which depends on the choice of the boundary piece. For all other W the entropy production formally diverges.

Now we have $B = \sum \lambda_k X_k$ (compare Sect. III), where $\lambda_k \geqq 0$. The X_k are the extremal points of the set $\mathscr{C}[A]$. Hence we have $\mathrm{d}H/\mathrm{d}t \leqq 0$ for every master operator B (compare [4]). Thus we finally have

$$\mathrm{d}H/\mathrm{d}t = -\sqrt{b/2\sigma} \sum \log w_\nu (w_\nu - w_{s(\nu)}) < 0\,,$$

equality only occurs, if the condition (41) is fulfilled and the remaining $w_\nu \neq 0$ all are equal. In other words

$$\mathrm{d}H/\mathrm{d}t\,[W, B] < \mathrm{d}H/\mathrm{d}t\,[W, B^{\max}] \leqq 0\,, \qquad (42)$$

if $W \neq W^{\mathrm{eq}}$, $B \neq B^{\max}$. Note that $B^{\max}$ corresponds to a point $B \in \mathfrak{B}$ with *maximal* distance d from X ($\triangleq W$). Then we have with

$$\begin{aligned} K &= \{B' \mid B' \in \mathfrak{B} \wedge \| X - B' \| = d\}\,, \\ B' &= B + C\colon\ B' \in K \Rightarrow \| C \|^2 + 2\langle B - X, C\rangle \\ &= \| C \| (\| C \| + 2 \| B - X \| \cos\alpha) = 0\,. \end{aligned}$$

Hence

$$\| C \| \neq 0 \;\Rightarrow\; \cos\alpha = -\| C \|/2\mathrm{d}\,.$$

Thus we get

$$\| C \| \to 0 \;\Rightarrow\; \cos\alpha \to 0\,.$$

But then B is an analytical extremum and therefore a *minimum*. Therefore $\| C \| = 0$. Hence only isolated points in $\mathfrak{B}$ can have maximal distance from X, and only extremal points can occur. If any inner point occurred, then we would have an analytical maximum which is impossible.

Let us make two remarks:

1) We consider the mapping T: $T(\nu) = S(\nu)$ (compare (38)). Of course this mapping is one to one, hence it is a permutation. If T maps the set $A = \{\alpha / w_\alpha = 0\}$ onto itself and if there are at least two $w_\beta \neq 0$, then there exists a statistical operator W which fulfills condition (41).

2) Let us consider a solution $\{\tilde{w}_\nu = \text{const}, \tilde{w}_\mu = 0\}$ The corresponding W then is stationary. The equation of motion reads

$$\begin{aligned} s_\nu \dot{w}_\nu &= \sum B_{\nu\mu} w_\mu \\ &= B_{\nu\nu} w_\nu + B_{\nu s(\nu)} w_{s(\nu)} = 0 \quad \text{for all } \nu. \end{aligned}$$

Thus we have obtained additional integrals of motion, if the master operator B determines a permutation which can be decomposed into non-trivial cycles.

VI. Summary

We have shown that all analytical extremal operators yield minima of the entropy production $\mathrm{d}H/\mathrm{d}t$. No minimum exists in $\mathring{\mathfrak{B}}$ and no minimum exists for η with

$$\eta_{\nu\mu} = \begin{Bmatrix} 1 \mid \nu \neq i,\ \mu \neq j \\ 0 \mid \nu = i,\ \mu = j \end{Bmatrix}.$$

On the other hand, a solution exists for the matrix η given by Equation (27). Using the theorem in Sect. III we see that a general insolvability theorem is not valid. Thus the general question remains open, which matrices η lead to solutions and for which statistical operators W, then, solutions do exist. All maxima correspond to extremal points and we have

$$\mathrm{d}H/\mathrm{d}t\,[W, B] < \mathrm{d}H/\mathrm{d}t\,[W, B^{\max}] \leqq 0 \quad \text{for} \quad W \neq W^{\mathrm{eq}}\,.$$

Thus, for $W \neq W^{\mathrm{eq}}$ and for any master operator B which has no zero matrix elements, we have that the entropy production $\mathrm{d}H/\mathrm{d}t < 0$. Question: Are these results true again for the case that the space $\mathfrak{S}$ contains non-commuting operators A_i?

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