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A theorem on Lyapunov stability for dynamical systems and a conjecture on a property of entropy

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For a general dynamical system, it is proved that an equilibrium state belonging to a continuous family of conditionally stable equilibrium states is stable. The result is applied to quantum thermodynamics to clarify in what restricted sense the entropy functional $s(\rho) = -k \operatorname{Tr} \rho \ln \rho$ can provide a Lyapunov criterion for the stability of thermodynamic equilibrium. A conjecture on a special positive-definiteness property of $-k \operatorname{Tr} \rho \ln \rho$ remains to be proved.

I. INTRODUCTION

In this note we address the question of whether entropy is indeed a Lyapunov function of the kind often implied in some thermodynamics literature on the stability of the maximum entropy equilibrium states.[1]

For a general dynamical system,[2] we call L functions those Lyapunov functions[3] that satisfy the hypothesis of Lyapunov's stability theorem.[4] We also define a special class of nondecreasing functions, called S functions, that satisfy the hypothesis of a conditional stability theorem. We prove a theorem giving a sufficient condition for the stability of equilibrium: an equilibrium state is stable if it belongs to a continuous family of conditionally stable equilibrium states (Theorem 3).

We apply the theorem to quantum thermodynamics to clarify the open question whether the entropy functional $s(\rho) = -k \operatorname{Tr} \rho \ln \rho$, together with the principle of nondecrease of entropy, indeed provides a Lyapunov criterion for the stability of thermodynamic equilibrium. We show that $s(\rho)$ is not an L function. We conjecture (Sec. III) that $s(\rho)$ is an S function, but provide only heuristic arguments in support of the conjecture. Thus, the open question remains unresolved, and calls for a technical study of the conjecture.

In view of our result, statements to the effect that the second law of thermodynamics "can be formulated as a dynamical principle in terms of the existence of a Lyapunov variable,[1]" should be taken *cum grano salis*, for they are either unnecessarily strong, if by Lyapunov variable is meant an L function,[1] or too weak, if by Lyapunov function is meant an S function.

Section II presents the general context of the problem. Section III presents its application to quantum thermodynamics.

II. *L* FUNCTIONS AND *S* FUNCTIONS

Definition 1: A *dynamical system*[2] on a metric space $(\mathscr{X}, d)$ is a mapping u: $\mathbb{R}^+ \times \mathscr{X} \to \mathscr{X}$ such that

(1.1) $u(\cdot, x)$: $\mathbb{R}^+ \to \mathscr{X}$ is continuous;
(1.2) $u(t, \cdot)$: $\mathscr{X} \to \mathscr{X}$ is continuous;
(1.3) $u(0, x) = x$;
(1.4) $u(t+s, x) = u(t, u(s, x))$;

for all t, s in $\mathbb{R}^+$, and x in $\mathscr{X}$.

The mapping $u(\cdot,x)$ is called the *motion* passing through x at time $t=0$. The set $\mathscr{X}$ is also called the *state space*, and $u(t,x)$ is the *state* at time t for a motion passing through state x at time 0. A part of a motion $u(\cdot,x)$ over an interval $[t_1,t_2]$ in $\mathbb{R}^+$, $t_2 > t_1$, with $u(t_1,x) = x_1$ and $u(t_2,x) = x_2$, is called a *process from* state x_1 *to* state x_2.[5] The metric d: $\mathscr{X} \times \mathscr{X} \to \mathbb{R}$ is such that $d(x,y) = 0$ if and only if $x = y$, $d(x,y) = d(y,x) \geqslant 0$, and $d(x,y) + d(y,z) \geqslant d(x,z)$ for all x, y, z in $\mathscr{X}$.

The dynamical system is determined by a one-parameter *semigroup* $\Lambda(t)$: $\mathscr{X} \to \mathscr{X}$ such that $\Lambda(t)x = u(t,x)$ for all t in $\mathbb{R}^+$ and x in $\mathscr{X}$, and that the inverse $\Lambda(t)^{-1}$ does not necessarily exist, so that the semigroup may not be extendable to a group with $\Lambda(-t) = \Lambda(t)^{-1}$.

Definition 2: A state x_e is an *equilibrium state* if and only if $u(t, x_e) = x_e$ for all t in $\mathbb{R}^+$.

Next, we recall the definitions of stability and instability according to Lyapunov. We will use the term local stability instead of Lyapunov stability to leave room for nonlocal stability concepts, such as that of metastability.[6]

Definition 3: An equilibrium state x_e is *locally stable* if and only if for each $\epsilon > 0$ there is a $\delta(\epsilon) > 0$ such that $d(x,x_e) < \delta(\epsilon)$ implies $d(u(t,x),x_e) < \epsilon$ for all $t > 0$ and every x in $\mathscr{X}$.

Definition 4: An equilibrium state x_e is *unstable* if and only if it is not locally stable, i.e., there is an $\epsilon > 0$ such that for every $\delta > 0$ there is a $t > 0$ and an x in $\mathscr{X}$ with $d(x,x_e) < \delta$ such that $d(u(t,x),x_e) \geqslant \epsilon$.

For any $r > 0$, $\mathscr{B}_r(x_e)$ will denote any open neighborhood of x_e containing the open ball with radius r and center x_e, i.e., all the states x such that $d(x,x_e) < r$.

Definition 5: A function $L(\cdot)$: $\mathscr{X} \to \mathbb{R}$ is an *L function* on an open neighborhood $\mathscr{B}_r(x_e)$ of an equilibrium state x_e if and only if the following conditions hold.

(5.1) $L(x) - L(x_e) \geqslant a(d(x,x_e))$ for every x in $\mathscr{B}_r(x_e)$ and some function $a(\cdot)$: $\mathbb{R} \to \mathbb{R}$ such that $a(0) = 0$, $\epsilon > 0$ implies $a(\epsilon) > 0$, and $a(r) < a(s)$ implies $r < s$.

(5.2) $L(u(t,x)) \leqslant L(x)$ for all $t > 0$ and every x in $\mathscr{B}_r(x_e)$.

(5.3) $L(\cdot)$: $\mathscr{X} \to \mathbb{R}$ is continuous at x_e, i.e., for each $\zeta > 0$ there is a $\delta'(\zeta) > 0$ such that $|L(x) - L(x_e)| < \zeta$ for every x in $\mathscr{X}$ with $d(x,x_e) < \delta'(\zeta)$.

L functions are the special class of Lyapunov functions[3] considered in the hypothesis of the classical Lyapunov stability theorem.[4]

Theorem 1. Lyapunov Stability Theorem: If $L(\cdot)$: $\mathscr{X} \to \mathbb{R}$ is an L function on an open neighborhood $\mathscr{B}_r(x_e)$ of an equilibrium state x_e, then x_e is a locally stable equilibrium state.

Proof: For each $\epsilon > 0$ (we may suppose $\epsilon < r$ with no loss of generality), let $\zeta(\epsilon) = a(\epsilon) > 0$, where $a(\cdot)$ is the function in

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condition (5.1). By conditions (5.3) and (5.1), there is a $\delta(\epsilon)=\delta'(\zeta(\epsilon))>0$ such that $L(x)-L(x_e)<a(\epsilon)$ for every x with $d(x,x_e)<\delta(\epsilon)$. By conditions (5.1) and (5.2),

$$a(d(u(t,x),x_e))\leqslant L(u(x,t))-L(x_e)\leqslant L(x)-L(x_e)<a(\epsilon), \tag{1}$$

for every $t>0$ and, hence, $d(u(t,x),x_e)<\epsilon$, i.e., x_e satisfies Definition 3. Thus, Theorem 1 is proved.

Definition 6: A single-valued function $E(\cdot)$: $\mathscr{X}\to\mathbb{R}^k$ is an *invariant* if and only if $E(u(t,x))=E(x)$ for all t in $\mathbb{R}^+$ and every x in $\mathscr{X}$.

Definition 7: A subset $\mathscr{C}(E)$ of $\mathscr{X}$ is a *constant-E subset* if and only if $E(x)=E$ for all x in $\mathscr{C}(E)$ and $E(\cdot)$ is an invariant.

Clearly, $\mathscr{C}(E)$ coincides with $\mathscr{X}$ if $E(\cdot)$ is a trivial invariant, e.g., the constant functions $E(\cdot)=E$. If $E(\cdot)$ is a nontrivial invariant with a range R_E in $\mathbb{R}^k$, then each x in $\mathscr{X}$ belongs to one and only one constant-E subset $\mathscr{C}(E(x))$ and every motion $u(\cdot,x)$ lies entirely in $\mathscr{C}(E(x))$, i.e., $u(t,x)$ is in $\mathscr{C}(E(x))$ for all t in $\mathbb{R}^+$.

Definition 8: An equilibrium state x_e is *conditionally locally stable* with respect to an invariant $E(\cdot)$ if and only if for each $\eta>0$ there is a $\delta(\eta)>0$ such that $d(x,x_e)<\delta(\eta)$ implies $d(u(t,x),x_e)<\eta$ for all $t>0$ and every x in $\mathscr{C}(E(x_e))$.

A conditionally locally stable equilibrium state x_e [with respect to a nontrivial invariant $E(\cdot)$] is not necessarily also locally stable because stability with respect to "perturbations" that bring the state off the constant-E subset $\mathscr{C}(E(x_e))$ is not guaranteed by Definition 8.

For any $r>0$, $\mathscr{D}_r(x_e)$ will denote any constant-E neighborhood of x_e containing the open disk in $\mathscr{C}(E(x_e))$ with radius r and center x_e, i.e., all the states x such that $d(x,x_e)<r$ and $E(x)=E(x_e)$.

Definition 9: A function $S(\cdot)$: $\mathscr{C}(E(x_e))\to\mathbb{R}$ is an *S function* on a constant-E neighborhood $\mathscr{D}_r(x_e)$ of an equilibrium state x_e if and only if the following conditions hold.

(9.1) $S(x_e)-S(x)\geqslant a(d(x,x_e))$ for every x in $\mathscr{D}_r(x_e)$ and some function $a(\cdot)$: $\mathbb{R}\to\mathbb{R}$ such that $a(0)=0$, $\epsilon>0$ implies $a(\epsilon)>0$, and $a(r)<a(s)$ implies $r<s$.

(9.2) $S(u(t,x))\geqslant S(x)$ for all $t>0$ and every x in $\mathscr{D}_r(x_e)$.

(9.3) $S(\cdot)$: $\mathscr{C}(E(x_e))\to\mathbb{R}$ is continuous at x_e, i.e., for each $\zeta>0$ there is a $\delta'(\zeta)>0$ such that $|S(x_e)-S(x)|<\zeta$ for every x in $\mathscr{C}(E(x_e))$ with $d(x,x_e)<\delta'(\zeta)$.

S functions acquire importance in view of the following conditional stability theorem.

Theorem 2. Lyapunov Conditional Stability Theorem: If $S(\cdot)$: $\mathscr{C}(E(x_e))\to\mathbb{R}$ is an S function on a constant-E neighborhood $\mathscr{D}_r(x_e)$ of an equilibrium state x_e, then x_e is conditionally locally stable with respect to the invariant $E(\cdot)$.

The proof of this theorem is completely analogous to that of Theorem 1 and will not be repeated.

Clearly, if $L(\cdot)$ is an L function then $S(\cdot)=-L(\cdot)$ is an S function. However, the converse is not true necessarily, i.e., if $S(\cdot)$ is an S function, $L(\cdot)=-S(\cdot)$ is not necessarily an L function. For example, condition (9.1) holds only on a constant-E neighborhood of x_e, whereas condition (5.1) is required to hold on an unconstrained neighborhood of x_e.

For applications such as thermodynamics (see Sec. III), it may be easier to construct S functions than L functions. The following theorem gives a sufficient condition under which stability can be proved even if no L function can be found. The condition requires the existence of a continuous family of conditionally stable equilibrium states in the neighborhood of x_e.

Theorem 3: Given an equilibrium state x_e, if there exist an invariant $E(\cdot)$: $\mathscr{X}\to R_E$ and a single-valued family of equilibrium states $x_e(\cdot)$: $R_E\to\mathscr{X}$ such that the following conditions hold, then x_e is a stable equilibrium state.

(3.1) $E(\cdot)$ is continuous at x_e, and $E(x_e)=E_e$.

(3.2) $x_e(\cdot)$ is continuous at E_e, and $x_e(E_e)=x_e$.

(3.3) For some $\xi>0$, every $x_e(E)$ with $d(x_e(E),x_e)<\xi$ is conditionally locally stable with respect to the invariant $E(\cdot)$.

(3.3)′ For some $\xi>0$, there is an S function on a constant-E neighborhood of each equilibrium state $x_e(E)$ with $d(x_e(E),x_e)<\xi$.

By virtue of Theorem 2, conditions (3.3) and (3.3)′ are equivalent.

Proof: We must show that for each $\epsilon>0$ there is a $\delta(\epsilon)>0$ such that $d(x,x_e)<\delta(\epsilon)$ implies $d(u(t,x),x_e)<\epsilon$ for all $t>0$. Let $\epsilon>0$ be given. With no loss of generality, we may suppose $\epsilon<\xi$.

For each E such that $d(x_e(E),x_e)<\epsilon/2$, we define

$$\eta(\epsilon,E)=\inf\{d(x,x_e(E))|E(x)=E,\ d(x,x_e)\geqslant\epsilon\} \tag{2}$$

so that $E(x)=E$ and $d(x,x_e(E))<\eta(\epsilon,E)$, i.e., $d(x,x_e(E(x)))<\eta(\epsilon,E(x))$, implies $d(x,x_e)<\epsilon$, because $d(x,x_e)\geqslant\epsilon$ would imply $d(x,x_e(E))\geqslant\eta(\epsilon,E)$. Moreover, $\eta(\epsilon,E)>0$ because the triangular inequality $d(x,x_e(E))+d(x_e(E),x_e)\geqslant d(x,x_e)$, for each x with $E(x)=E$ and $d(x,x_e)\geqslant\epsilon$, implies $d(x,x_e(E))\geqslant\epsilon-\epsilon/2=\epsilon/2$, but $\eta(\epsilon,E)$ is the greatest lower bound of $d(x,x_e(E))$ and, therefore, $\eta(\epsilon,E)\geqslant\epsilon/2>0$.

Because $x_e(E)$ is conditionally stable (Condition 3.3), there is a $\delta(\eta(\epsilon,E))>0$ such that $E(x)=E$ and $d(x,x_e(E))<\delta(\eta(\epsilon,E))$ imply $d(u(t,x),x_e(E))<\eta(\epsilon,E)$ for all $t>0$ (Definition 8). We denote by $\delta(\epsilon,E)$ the lowest upper bound of all the δ's that satisfy Definition 8 for a given $\eta(\epsilon,E)$, i.e., $\delta(\epsilon,E)=\inf\{\delta(\eta(\epsilon,E))\}$, and we define

$$\gamma'(\epsilon)=\inf\{\delta(\epsilon,E)|E \text{ such that } d(x_e(E),x_e)<\epsilon/2\}, \tag{3}$$

so that $\delta(\epsilon,E)\geqslant\gamma'(\epsilon)\geqslant\delta(\eta(\epsilon,E))>0$ because $\gamma'(\epsilon)$ is the greatest lower bound of $\delta(\epsilon,E)$.

We now let $\gamma(\epsilon)=\min\{\epsilon,\gamma'(\epsilon)\}$ and define

$$\delta'(\epsilon)=\inf\{d(x,x_e)|d(x,x_e(E(x)))\geqslant\gamma(\epsilon),$$
$$d(x_e(E(x)),x_e)<\gamma(\epsilon)/2\}, \tag{4}$$

so that $d(x,x_e)<\delta'(\epsilon)$ and $d(x_e(E(x)),x_e)<\gamma(\epsilon)/2$ imply $d(x,x_e(E(x)))<\gamma(\epsilon)$ because $d(x,x_e(E(x)))\geqslant\gamma(\epsilon)$ would imply $d(x,x_e)\geqslant\delta'(\epsilon)$. Moreover, $\delta'(\epsilon)>0$ because the triangular inequality $d(x,x_e)+d(x_e(E(x)),x_e)\geqslant d(x,x_e(E(x)))$, for each x with $d(x,x_e(E(x)))\geqslant\gamma(\epsilon)$ and $d(x_e(E(x)),x_e)<\gamma(\epsilon)/2$, implies $d(x,x_e)\geqslant\gamma(\epsilon)-\gamma(\epsilon)/2=\gamma(\epsilon)$, but $\delta'(\epsilon)$ is the greatest lower bound of $d(x,x_e)$ and, therefore, $\delta'(\epsilon)\geqslant\gamma(\epsilon)/2>0$.

Because of conditions (3.1) and (3.2), $x_e(E(\cdot))$ is continuous at x_e and, therefore, there is a $\delta''(\epsilon)>0$ such that $d(x,x_e)<\delta''(\epsilon)$ implies $d(x_e(E(x)),x_e)<\gamma(\epsilon)/2$. If we now let $\delta(\epsilon)=\min\{\delta''(\epsilon),\delta'(\epsilon)\}$, then $d(x,x_e)<\delta(\epsilon)$ implies $d(x_e(E(x)),x_e)<\gamma(\epsilon)/2\leqslant\epsilon/2$ and $d(x,x_e(E(x)))<\gamma(\epsilon)\leqslant\gamma'(\epsilon)\leqslant\delta(\epsilon,E(x))$. Therefore, $d(u(t,x),x_e(E(x)))<\eta(\epsilon,E(x))$ and $d(u(t,x),x_e)<\epsilon$. Thus, Theorem 3 is proved.

III. APPLICATION TO QUANTUM THERMODYNAMICS

Within quantum theory, Theorem 3 is immediately applicable to study the stability of equilibria of (possibly nonlinear) generalized evolution equations for irreversible dynamics.

Let us consider an isolated physical system with associated Hilbert space $\mathscr{H}$ (dim $\mathscr{H} \leqslant \infty$), and Hamiltonian operator H (possibly unbounded). For simplicity, let the number operators N_i for each type i of elementary constituent be c-number operators, i.e., $N_i = \text{N}_i I$. If H is unbounded, we further assume that $\text{Tr} \exp(-\beta H) < \infty$ for all β with $0 < \beta < \infty$,[7] and that the energy functional

$$E(\rho) = \text{Tr}\, H\rho \tag{5}$$

is continuous[7] on the set of self-adjoint, non-negative-definite, unit-trace operators on $\mathscr{H}$ with respect to the metric $d(\rho_1, \rho_2) = \text{Tr}|\rho_1 - \rho_2|$.

We then define the *state space* $\mathscr{L}_c$ to be the set of all self-adjoint, non-negative-definite, unit-trace operators ρ on $\mathscr{H}$ with energy $\text{Tr}\, H\rho \leqslant c$, with c a given finite constant, i.e.,

$$\mathscr{L}_c = \{ \rho \text{ on } \mathscr{H} | \rho^\dagger = \rho, \quad \rho \geqslant 0,\ \text{Tr}\,\rho = 1,\ \text{Tr}\, H\rho \leqslant c < \infty \}. \tag{6}$$

Operators ρ are called *state operators* for, within quantum thermodynamics, they represent the states of the physical system.

The entropy functional

$$s(\rho) = -k \,\text{Tr}\,\rho \ln \rho \tag{7}$$

is concave[8] and continuous[9] on $\mathscr{L}_c$. Moreover, for a given value E in the range R_E, i.e., for

$$\inf\{E(\rho)|\rho \text{ in } \mathscr{L}_c\} < E < \sup\{E(\rho)|\rho \text{ in } \mathscr{L}_c\} \tag{8}$$

the entropy functional $s(\rho)$ has a unique maximum on the set

$$\mathscr{C}(E) = \{\rho \text{ in } \mathscr{L}_c | E(\rho) = E\} \tag{9}$$

at the state

$$\rho_0(E) = \exp(-\beta(E)H)/\text{Tr}\exp(-\beta(E)H), \tag{10}$$

where $\beta(E)$ is one-to-one and continuous in the specified range for E (see Refs. 10 and 11). Namely $s(\rho_0(E)) > s(\rho)$ for every $\rho \neq \rho_0(E)$ in $\mathscr{C}(E)$. Thus, the family of states $\rho_0(E)$ is single valued and continuous in E.

Now, let us assume that the causal evolution of state operators forms a *dynamical system* on $(\mathscr{L}_c, d)$ such that the energy functional is a nontrivial invariant and the entropy functional is nondecreasing, i.e., for every ρ in $\mathscr{L}_c$ the motion $u(\cdot,\rho)$ is such that

$$E(u(t,\rho)) = E(\rho), \tag{11}$$

$$s(u(t,\rho)) \geqslant s(\rho), \tag{12}$$

for all $t \geqslant 0$.

Consider a state $\rho_0(E)$ [Eq. (10)]. Because $E(\rho)$ is an invariant, $u(t,\rho_0(E))$ is in $\mathscr{C}(E)$ for every $t \geqslant 0$. Because $s(\rho)$ is nondecreasing, $s(u(t,\rho_0(E))) \geqslant s(\rho_0(E))$ for every $t \geqslant 0$. But $s(\rho) < s(\rho_0(E))$ for every $\rho \neq \rho_0(E)$ in $\mathscr{C}(E)$. Therefore, $u(t,\rho_0(E)) = \rho_0(E)$, i.e., each $\rho_0(E)$ is an equilibrium state (Definition 2). We conclude that conditions (3.1), (3.2), and (3.3) of Theorem 3 are satisfied for each equilibrium state $\rho_0(E)$. If each such equilibrium state were shown to be conditionally locally stable then it would also be locally stable by virtue of Theorem 3.

It is noteworthy that, because in any neighborhood of every equilibrium state $\rho_0(E)$ [excluding the state with $E = c$ and the state with $\beta(E) = 0$, if H is bounded] there is another state $\rho_0(E')$ such that $s(\rho_0(E')) > s(\rho_0(E))$, the functions $L_1(\cdot) = -s(\cdot)$ and $L_2(\cdot) = s(\rho_0(E(\cdot))) - s(\cdot)$ are not L functions on any neighborhood of any stable equilibrium state in $\mathscr{L}_c$ with entropy less than the absolute maximum on $\mathscr{L}_c$. Indeed, we could have $L_1(\rho_0(E')) - L_1(\rho_0(E)) < 0$ and $L_2(\rho_0(E')) - L_2(\rho_0(E)) = 0$ even though $d(\rho_0(E'),\rho_0(E)) > 0$ and, therefore, neither $L_1(\cdot)$ nor $L_2(\cdot)$ could satisfy condition (5.1).

The physical importance of showing that the maximum entropy equilibrium states are locally stable emerges from the second law of thermodynamics which requires them to be the only (locally) stable equilibrium states.[12] For the dynamical system to be consistent with the second law of thermodynamics, it must necessarily imply that the maximum entropy equilibrium states are locally stable, and that any other equilibrium state is unstable.

For example, a unitary (Hamiltonian) dynamical system with $u(t,\rho) = U(t)\rho U(t)^{-1}$, $U(t) = \exp(-iH/\hbar)$, would satisfy conditions (11) and (12) with $s(u(t,\rho)) = s(\rho)$. However, it would imply the existence of other stable equilibrium states in addition to those with maximum entropy for a given energy E. Indeed, every equilibrium state ρ_e of such a dynamical system, i.e., every state operator with $\rho_e H = H\rho_e$, would be locally stable because $d(u(t,\rho),\rho_e) = d(\rho,\rho_e)$ for all t and every ρ, i.e., each motion would remain at a fixed distance from every equilibrium state,[13] and, therefore, Definition 3 would be satisfied for each $\epsilon > 0$ with $\delta(\epsilon) = \epsilon$. Thus, a unitary (Hamiltonian) dynamical system would not be consistent with the second law of thermodynamics.

In general, the existence of *dissipative* motions, i.e., motions with $s(u(t,\rho)) > s(\rho)$ for some $t > 0$, reduces both the number of equilibrium states and the number of equilibrium states that are stable. For example, the dynamical system generated by the nonlinear evolution equation recently proposed by the author in the framework of quantum thermodynamics[14,15] not only satisfies conditions (11) and (12), but seems also to contain enough dissipative motions to imply that only the maximum entropy equilibrium states are locally stable, whereas the many other equilibrium states are all unstable, which is consistent with the second law of thermodynamics.

This paper addresses only the question of whether the principle of nondecrease of entropy [condition (12)], together with the properties of the entropy functional [Eq. (7)] and the specific structure of the maximum entropy states [Eq. (10)], is sufficient to imply the local stability of the maximum entropy thermodynamic equilibrium states. In view of Theorem 3, we concluded that it would suffice to show that the entropy functional is an S function and, specifically, that it satisfies condition (9.1) for each equilibrium state $\rho_0(E)$.

In some thermodynamic literature, it is usually stated that entropy provides a Lyapunov criterion for the stability of the thermodynamic equilibrium states.[1,16] However, a rigorous justification of these assertions is found nowhere in the literature.

The question would be resolved if we could prove that the functional $s(\rho_0(E)) - s(\rho)$, when restricted to the constant-E subset containing $\rho_0(E)$, is positive definite in the sense made precise by the conjecture below. If the conjecture could be proved, then condition (9.1) would be satisfied, entropy would be an S function in the neighborhood of each maximum entropy equilibrium state, and Theorem 3 would guarantee the local stability of such states. Only then, and in the strict sense specified here, would it be correct to aver that entropy provides a Lyapunov criterion for the stability of thermodynamic equilibrium.

Conjecture: Given a state operator of the form

$$\rho_0 = \frac{\exp(-\Sigma_j \lambda_j R_j)}{\operatorname{Tr}\exp(-\Sigma_i \lambda_i R_i)}, \tag{13}$$

such that $\operatorname{Tr}\exp(-\Sigma_j \lambda_j R_j) < \infty$, there is a function $a(\cdot)$: $\mathbb{R}\rightarrow\mathbb{R}$ such that $a(0) = 0$, $\epsilon > 0$ implies $a(\epsilon) > 0$, $a(r) < a(s)$ implies $r < s$, and

$$\operatorname{Tr}\rho\ln\rho - \operatorname{Tr}\rho_0\ln\rho_0 \geqslant a(\operatorname{Tr}|\rho - \rho_0|), \tag{14}$$

for every state operator ρ such that $\operatorname{Tr} R_j\rho = \operatorname{Tr} R_j\rho_0$ for every j, and $\operatorname{Tr}|\rho - \rho_0| < \xi$ for some $\xi > 0$.

We have no proof of this conjecture. But its validity seems to be plausible in view of the following facts: (1) state operator ρ_0 is the unique state maximizing $-\operatorname{Tr}\rho\ln\rho$ over the set of states with $\operatorname{Tr} R_j\rho = \operatorname{Tr} R_j\rho_0$; (2) $-\operatorname{Tr}\rho\ln\rho$ is continuous in ρ_0 (see Ref. 9); (3) $-\operatorname{Tr}\rho\ln\rho$ is strictly concave (see Ref. 8); and (4) state operator ρ_0 is strictly positive. Heuristically, there should be a way to expand the functional $-\operatorname{Tr}\rho\ln\rho$ (restricted over the set with $\operatorname{Tr} R_j\rho = \operatorname{Tr} R_j\rho_0$) in a Taylor series about ρ_0 to find

$$-\operatorname{Tr}\rho\ln\rho = -\operatorname{Tr}\rho_0\ln\rho_0 + D_1\operatorname{Tr}(\rho - \rho_0) + D_2\operatorname{Tr}(\rho - \rho_0)^2 + \cdots . \tag{15}$$

Then, D_1 should equal zero because ρ_0 maximizes $-\operatorname{Tr}\rho\ln\rho$ over the restricted set, and D_2 should be defined and strictly negative because ρ_0 is strictly positive and $-\operatorname{Tr}\rho\ln\rho$ is strictly concave. A proof on these lines, however, would involve several technical problems of the kind discussed in Ref. 8, such as the essential singularity of function $-y\ln y$ at $y = 0$, the delicate question of continuity of $-\operatorname{Tr}\rho\ln\rho$, the question of differentiability of $-\operatorname{Tr}\rho\ln\rho$, and so on.

We hope that the arguments just outlined in support of the conjecture will provide sufficient motivation for a rigorous technical study that would settle an important open question in the field of thermodynamics.

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[2] See, e.g., J. A. Walker, *Dynamical Systems and Evolution Equations* (Plenum, New York, 1980), p. 86, and references therein.

[3] See, e.g., Ref. 2, p. 138.

[4] See, e.g., Ref. 2, p. 157.

[5] A given process from state x_1 to state x_2 is *reversible* if and only if in the dynamical system there is a process from x_2 to x_1, i.e., the dynamical system contains a "restoring" motion $u(\cdot,x_r)$ such that $u(t',x_r) = x_2$ and $u(t'',x_r) = x_1$ with $t'' > t'$. Otherwise, the process from x_1 to x_2 is *irreversible*. It is noteworthy that if a motion $u(\cdot,x)$ gives rise to a reversible process then the motion is periodic, i.e., there is a $t > 0$ such that $u(t,x) = x$. Clearly, should there be a function $S(\cdot)$: $\mathscr{X}\rightarrow\mathbb{R}$ such that $S(u(t,x)) \geqslant S(x)$ for all x in $\mathscr{X}$ and t in $\mathbb{R}^+$, then any process from x_1 to x_2 with $S(x_2) > S(x_1)$ would be irreversible.

[6] We have not found clear definitions of the concepts of metastability and global stability of the equilibrium states of a dynamical system anywhere in the literature. These definitions would be of much importance in the thermodynamics framework described in Sec. III, however, they are not needed in this paper.

[7] These conditions are, in general, more restrictive than necessary. See, Refs. 8 and 10.

[8] A. Wehrl, Rev. Mod. Phys. **50**, 221 (1978).

[9] Reference 8, p. 241.

[10] W. Ochs and W. Bayer, Z. Naturforsch **28a**, 693, 1571 (1973).

[11] A. Katz, *Principles of Statistical Mechanics* (Freeman, San Francisco, 1967), pp. 45–51.

[12] G. N. Hatsopoulos and J. H. Keenan, *Principles of General Thermodynamics* (Wiley, New York, 1965), pp. 367–373; G. N. Hatsopoulos and E. P. Gyftopoulos, Found. Phys. **6**, 15, 127, 439, 561 (1976).

[13] $d(u(t,\rho),\rho_e) = \operatorname{Tr}|U(t)\rho U(t)^{-1} - \rho_e| = \operatorname{Tr} U(t)|\rho - \rho_e|U(t)^{-1} = \operatorname{Tr}|\rho - \rho_e| = d(\rho,\rho_e)$ for every ρ and each ρ_e such that $\rho_e U(t) = U(t)\rho_e$.

[14] G. P. Beretta, Sc.D. thesis, M.I.T., 1981 (unpublished); G. P. Beretta, E. P. Gyftopoulos, J. L. Park, and G. N. Hatsopoulos, Nuovo Cimento B **82**, 169 (1984); G. P. Beretta, E. P. Gyftopoulos, and J. L. Park, Nuovo Cimento B **87**, 77 (1985).

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[16] See also R. F. Fox, Proc. Natl. Acad. Sci. USA **77**, 3763 (1980), where some assertions in Ref. 1 regarding Lyapunov functions for steady nonequilibrium states are criticized, but their validity near equilibrium is not questioned.