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A System-Theoretic Foundation for Thermodynamics: Energy Flow, Energy Balance, Energy Equipartition, Entropy, and Ectropy

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***Abstract*— Thermodynamics is a physical branch of science that governs the thermal behavior of dynamical systems as simple as refrigerators to as complex as our expanding universe. The development of thermodynamics spawned out of steam tables and venous bleeding with many scientists and engineers expressing concerns about the completeness and clarity of its mathematical exposition over its tortuous history. In this paper we develop a system-theoretic foundation for thermodynamics using a large-scale dynamical systems perspective. Specifically, using compartmental dynamical system energy flow models, we place the universal energy conservation, energy equipartition, temperature equipartition, and entropy nonconservation laws of thermodynamics on a system-theoretic foundation. Furthermore, we introduce a *new* and dual notion to entropy; namely, *ectropy*, as a measure of the tendency of a dynamical system to do useful work and show that conservation of energy in an isolated thermodynamic system necessarily leads to nonconservation of ectropy and entropy. In addition, using the system ectropy as a Lyapunov function candidate we show that our large-scale thermodynamic energy flow model has convergent trajectories to Lyapunov stable equilibria determined by the large-scale system initial subsystem energies.**

I. INTRODUCTION

Energy is a concept that underlies our understanding of all physical phenomena and is a measure of the ability of a dynamical system to produce changes (motion) in its own system state as well as changes in the system states of its surroundings. Thermodynamics is a physical branch of science that deals with laws governing energy flow from one body to another and energy transformations from one form to another. These energy flow laws are captured by the fundamental principles known as the first and second laws of thermodynamics. The first law of thermodynamics gives a precise formulation of the equivalence of heat and work and states that among all system transformations, the net system energy is conserved. Hence, energy cannot be created out of nothing and cannot be destroyed, merely transferred from one form to another. The law of conservation of energy is not a mathematical truth, but rather the consequence of an immeasurable culmination of observations over the chronicle of our civilization and is a fundamental *axiom* of the science of heat. The first law does not tell us whether any particular process can actually occur; that is, it does not restrict the ability to convert work into heat or heat into work, except that energy must be conserved in the process. The second law of thermodynamics asserts that while the system energy is always conserved, it will be degraded to a point where it cannot produce any useful work. Hence, it is impossible to extract work from heat without at the same time discarding some heat giving rise to a monotonically increasing quantity known as *entropy*. While energy describes the state of a dynamical system, entropy refers to changes in the *status quo* of the system and is a measure of molecular disorder and the amount of wasted energy in a dynamical (energy) transformation from one state (form) to another. Since the system entropy monotonically increases, the entropy of the dynamical system tends to a maximum and thus time, as determined by system entropy increase [1–3], flows on in one direction only. Even though entropy is a physical property of matter which is not directly observable, it permeates the whole of nature, regulating the *arrow of time* and responsible for the enfeeblement and eventual demise of the universe. While the laws of thermodynamics form the foundation to basic engineering systems as well as nuclear explosions, cosmology, and our expanding universe, many engineers and scientists have expressed concerns about the completeness and clarity of the different expositions of thermodynamics over its long and flexuous history, see [4–12].

Since the specific motion of every molecule of a thermodynamic system is impossible to predict, a *macroscopic* model of the system is typically used with appropriate macroscopic states which include pressure, volume, temperature, internal energy, and entropy, among others. However, a thermodynamically consistent energy flow model should ensure that the system energy can be modelled by a diffusion (conservation) equation in the form of a *parabolic* partial differential equation. These systems are infinite-dimensional and hence finite-dimensional approximations are of very high order giving rise to large-scale dynamical systems. Since energy is a fundamental concept in the analysis of large-scale dynamical systems and heat (energy) is a fundamental concept of thermodynamics involving the capacity of hot bodies (more energetic subsystems) to produce work, thermodynamics is a theory of large-scale dynamical systems. High dimensional dynamical systems can arise from both macroscopic and *microscopic* points of view. Microscopic thermodynamic models can have the form of a distributed parameter model or a large-scale system model comprised of a large number of interconnected subsystems. In contrast to macroscopic models involving

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the evolution of global quantities (e.g., energy, temperature, entropy, etc.), microscopic models are based upon the modeling of local quantities that describe the atoms and molecules that make up the system, and their speeds, energies, masses, angular momenta, behavior during collisions, etc. The mathematical formulations based on these quantities form the basis of *statistical mechanics*. Since microscopic details are obscured on the macroscopic level, it is appropriate to view a microscopic model as an inherent model of uncertainty. However, for a thermodynamic system the macroscopic and microscopic quantities are related since they are simply different ways of describing the same phenomena. Thus, if the global macroscopic quantities can be expressed in terms of the local microscopic quantities, the laws of thermodynamics could be described in the language of statistical mechanics. This interweaving of the microscopic and macroscopic points of view lead to diffusion being a natural consequence of dimensionality and, hence, uncertainty on the microscopic level despite the fact that there is no uncertainty about the diffusion process per se.

In the last half of the 20th century thermodynamics was re-formulated as a global nonlinear field theory with the ultimate objective to determine the independent field variables of this theory [13–15]. This aspect of thermodynamics, which became known as *rational thermodynamics*, was predicated on an entirely new axiomatic approach. As a result of this approach, modern continuum thermodynamics was developed using theories from elastic materials, viscous materials, and materials with memory [16–19]. Connections between thermodynamics and system theory as well as information theory were also explored [20–27]. For an excellent exposition of these different facets of thermodynamics see [28]. Thermodynamic principles have also been repeatedly used in coupled mechanical systems to arrive at energy flow models with modal energy playing the role of temperature. Specifically, in an attempt to approximate high-dimensional dynamics of large-scale structural (oscillatory) systems with a low-dimensional diffusive (non-oscillatory) dynamical model, structural dynamicists have developed thermodynamic energy flow models using stochastic energy flow techniques. In particular, statistical energy analysis (SEA) predicated on averaging system states over the statistics of the uncertain system parameters has been extensively developed for mechanical and acoustic vibration problems [29–34]. Thermodynamic models are derived from large-scale dynamical systems of discrete subsystems involving stored energy flow among subsystems based on the assumption of weak subsystem coupling or identical subsystems. However, the ability of SEA to predict the dynamic behavior of a complex large-scale dynamical system in terms of pairwise subsystem interactions is severely limited by the coupling strength of the remaining subsystems on the subsystem pair. Hence, it is not surprising that SEA energy flow predictions for large-scale systems with strong coupling can be erroneous. Alternatively, a deterministic thermodynamically motivated energy flow modeling for structural systems is addressed in [35], [36]. This approach exploits energy flow models in terms of thermodynamic energy (i.e., ability to dissipate heat) as opposed to stored energy and is not limited to weak subsystem coupling. Finally, a stochastic energy flow compartmental model (i.e., a model characterized by conservation laws) predicated on averaging system states over the statistics of stochastic system exogenous disturbances is developed in [23]. The basic result demonstrates how linear compartmental models arise from second-moment analysis of state space systems under the assumption of weak coupling. Even though these results can be potentially applicable to linear large-scale dynamical systems with weak coupling, such connections are not explored in [23]. With the notable exception of [34], none of the aforementioned SEA-related works address the second law of thermodynamics involving entropy notions in the energy flow between subsystems.

The goal of the present paper is directed toward placing thermodynamics on a system-theoretic foundation. Specifically, since thermodynamic models are concerned with energy flow among subsystems, we develop a nonlinear compartmental dynamical system model that is characterized by energy conservation laws capturing the exchange of energy between coupled macroscopic subsystems. Furthermore, using graph theoretic notions we state two thermodynamic axioms consistent with the zeroth and second laws of thermodynamics that ensure that our large-scale dynamical system model gives rise to a thermodynamically consistent energy flow model. Specifically, using a large-scale dynamical systems theory perspective for thermodynamics, we show that our compartmental dynamical system model leads to a precise formulation of the equivalence between work energy and heat in a large-scale dynamical system. Next, we give a deterministic definition of entropy for a large-scale dynamical system that is consistent with the classical thermodynamic definition of entropy and show that it satisfies a Clausius-type inequality leading to the law of entropy nonconservation. Furthermore, we introduce a *new* and dual notion to entropy; namely, *ectropy*, as a measure of the tendency of a large-scale dynamical system to do useful work and show that conservation of energy in an isolated thermodynamically consistent system necessarily leads to nonconservation of ectropy and entropy. Then, using the system ectropy as a Lyapunov function candidate we show that our thermodynamically consistent large-scale nonlinear dynamical system model possesses a continuum of equilibria and is *semistable*; that is, it has convergent subsystem energies to Lyapunov stable energy equilibria determined by the large-scale system initial subsystem energies. In addition, we show that the steady-state distribution of the large-scale system energies is uniform leading to system energy equipartitioning corresponding to a minimum ectropy and a maximum entropy equilibrium state. In the case where the subsystem energies are proportional to subsystem temperatures, we show that our dynamical system model leads to temperature equipartition wherein all the system energy is transferred into heat at a uniform temperature. Furthermore, we show that our system-theoretic definition of entropy and the newly proposed notion of ectropy are consistent with Boltzmann's kinetic theory of gases involving an n-body theory of ideal gases divided by diathermal walls.

The contents of the paper are as follows. In Section II we establish notation, definitions, and review some basic results on nonnegative and compartmental dynamical systems. In Section III we use a large-scale dynamical systems perspective to provide a system-theoretic foundation for thermodynamics. Specifically, we develop a nonlinear compartmental dynamical model characterized by energy conservation laws that is consistent with the basic thermodynamic principles. Then we turn our attention to stability and convergence. In particular, using the total subsystem energies as a candidate system energy storage function, we show that our thermodynamic system is lossless and hence can deliver to its surroundings all of its stored subsystem energies and can store all of the work done to all of its subsystems. Next, using the system ectropy as a Lyapunov function candidate we show that the proposed thermodynamic model is semistable with a uniform energy distribution corresponding to a minimum ectropy and a maximum entropy. In Section IV we generalize the results of Section III to the case where the subsystem energies in large-scale dynamical system model are proportional to subsystem temperatures and arrive at temperature equipartition for the proposed thermodynamic model. Furthermore, we provide a kinetic theory interpretation of the steady-state expressions for entropy and ectropy. In Section V, we specialize the results of Section III to thermodynamic systems with linear energy exchange. In Section VI we extend the results of Section III to continuous thermodynamic systems wherein the subsystems are uniformly distributed over an n dimensional (not necessarily Euclidian) space. Specifically, we develop a nonlinear distributed parameter model wherein the system energy is modeled by a diffusion (conservation) equation in the form of a parabolic partial differential equation. Energy equipartition and semistability are shown using the well-known Sobolev embedding theorems and the notion of generalized (or weak) solutions. Finally, we draw conclusions in Section VII.

II. Mathematical Preliminaries

In this section we introduce notation, several definitions, and some key results needed for developing the main results of this paper. Let $\mathbb{R}$ denote the set of real numbers, $\mathbb{R}^n$ denote the set of $n \times 1$ column vectors, $(\cdot)^{\mathrm{T}}$ denote transpose, $(\cdot)^{\#}$ denote group generalized inverse, and let I_n or I denote the $n \times n$ identity matrix. For $v \in \mathbb{R}^q$ we write $v \geq\geq 0$ (respectively, $v >> 0$) to indicate that every component of v is nonnegative (respectively, positive). In this case we say that v is *nonnegative* or *positive*, respectively. Let $\overline{\mathbb{R}}_+^q$ and $\mathbb{R}_+^q$ denote the nonnegative and positive orthants of $\mathbb{R}^q$; that is, if $v \in \mathbb{R}^q$, then $v \in \overline{\mathbb{R}}_+^q$ and $v \in \mathbb{R}_+^q$ are equivalent, respectively, to $v \geq\geq 0$ and $v >> 0$. Furthermore, let $\partial\mathcal{S}$ and $\overline{\mathcal{S}}$ denote the boundary and the closure of the set $\mathcal{S}$, respectively. Finally, we write $\|\cdot\|$ for the Euclidean vector norm, $\|\cdot\|_{\mathcal{B}}$ for the operator norm of an element in a Banach space $\mathcal{B}$, $\mathcal{R}(M)$ for the range space of a matrix M, $V'(x)$ for the Fréchet derivative of V at x, $\mathcal{B}_\varepsilon(\alpha)$, $\alpha \in \mathbb{R}^n$, $\varepsilon > 0$, for the open ball centered at α with radius ε, $M \geq 0$ (respectively, $M > 0$) to denote the fact that the Hermitian matrix M is nonnegative (respectively, positive) definite, and $x(t) \to \mathcal{M}$ as $t \to \infty$ to denote that $x(t)$ approaches the set $\mathcal{M}$; that is, for each $\varepsilon > 0$ there exists $T > 0$ such that $\mathrm{dist}(x(t), \mathcal{M}) < \varepsilon$ for all $t > T$, where $\mathrm{dist}(p, \mathcal{M}) \triangleq \inf_{x\in\mathcal{M}} \|p - x\|_{\mathcal{B}}$. The following definition introduces the notion of Z-, M-, essentially nonnegative, compartmental, and nonnegative matrices.

Definition 2.1 ([23], [24], [37]): Let $W \in \mathbb{R}^{q\times q}$. W is a *Z-matrix* if $W_{(i,j)} \leq 0$, $i, j = 1, \ldots, q$, $i \neq j$. W is an *M-matrix* (respectively, a *nonsingular M-matrix*) if W is a Z-matrix and all the principal minors of W are nonnegative (respectively, positive). W is *essentially nonnegative* if $-W$ is a Z-matrix; that is, $W_{(i,j)} \geq 0$, $i, j = 1, \ldots, q$, $i \neq j$. W is *compartmental* if W is essentially nonnegative and $\sum_{i=1}^q W_{(i,j)} \leq 0$, $j = 1, ..., q$. Finally, W is *nonnegative*[1] (respectively, *positive*) if $W_{(i,j)} \geq 0$ (respectively, $W_{(i,j)} > 0$), $i, j = 1, \ldots, q$.

[1] In this paper it is important to distinguish between a square nonnegative (respectively, positive) matrix and a nonnegative-definite (respectively, positive-definite) matrix.

The following definition introduces the notion of essentially nonnegative functions [24], [38].

Definition 2.2: Let $w = [w_1, \cdots, w_q]^{\mathrm{T}} : \mathcal{V} \to \mathbb{R}^q$, where $\mathcal{V}$ is an open subset of $\mathbb{R}^q$ that contains $\overline{\mathbb{R}}_+^q$. Then w is *essentially nonnegative* if $w_i(z) \geq 0$ for all $i = 1, \ldots, q$ and $z \in \overline{\mathbb{R}}_+^q$ such that $z_i = 0$, where z_i denotes the ith component of z.

Note that if $w(z) = Wz$, where $W \in \mathbb{R}^{q\times q}$, then $w(\cdot)$ is essentially nonnegative if and only if W is an essentially nonnegative matrix.

Proposition 2.1 ([24], [38]): Suppose $\overline{\mathbb{R}}_+^q \subset \mathcal{V}$. Then $\overline{\mathbb{R}}_+^q$ is an invariant set with respect to

$$\dot{z}(t) = w(z(t)), \quad z(t_0) = z_0, \quad t \geq t_0, \tag{1}$$

where $z_0 \in \overline{\mathbb{R}}_+^q$, if and only if $w : \mathcal{V} \to \mathbb{R}^q$ is essentially nonnegative.

The following corollary to Proposition 2.1 is immediate.

Corollary 2.1: Let $W \in \mathbb{R}^{q\times q}$. Then W is essentially nonnegative if and only if e^{Wt} is nonnegative for all $t \geq 0$.

The following definition introduces several types of stability for the *nonnegative* dynamical system (1).

Definition 2.3: The equilibrium solution $z(t) \equiv z_{\mathrm{e}}$ of (1) is *Lyapunov stable* if, for every $\varepsilon > 0$, there exists $\delta = \delta(\varepsilon) > 0$ such that if $z_0 \in \mathcal{B}_\delta(z_{\mathrm{e}}) \cap \overline{\mathbb{R}}_+^q$, then $z(t) \in \mathcal{B}_\varepsilon(z_{\mathrm{e}}) \cap \overline{\mathbb{R}}_+^q$, $t \geq t_0$. The equilibrium solution $z(t) \equiv z_{\mathrm{e}}$ of (1) is *semistable* if it is Lyapunov stable and there exists $\delta > 0$ such that if $z_0 \in \mathcal{B}_\delta(z_{\mathrm{e}}) \cap \overline{\mathbb{R}}_+^q$, then $\lim_{t\to\infty} z(t)$ exists and converges to a Lyapunov stable equilibrium point. The equilibrium solution $z(t) \equiv z_{\mathrm{e}}$ of (1) is *asymptotically stable* if it is Lyapunov stable and there exists $\delta > 0$ such that if $z_0 \in \mathcal{B}_\delta(z_{\mathrm{e}}) \cap \overline{\mathbb{R}}_+^q$, then $\lim_{t\to\infty} z(t) = z_{\mathrm{e}}$. Finally, the equilibrium solution $z(t) \equiv z_{\mathrm{e}}$ of (1) is *globally asymptotically stable* if the previous statement holds for all $z_0 \in \overline{\mathbb{R}}_+^q$.

Finally, recall that a matrix $W \in \mathbb{R}^{q\times q}$ is *semistable* if and only if $\lim_{t\to\infty} e^{Wt}$ exists [23], [24] while W is *asymptotically stable* if and only if $\lim_{t\to\infty} e^{Wt} = 0$.

III. A System-Theoretic Foundation for Thermodynamics

The fundamental and unifying concept in the analysis of complex (large-scale) dynamical systems is the concept of energy. The energy of a state of a dynamical system is the measure of its ability to produce changes (motion) in its own system state as well as changes in the system states of its surroundings. These changes occur as a direct consequence of the energy flow between different subsystems within the dynamical system. Since heat (energy) is a fundamental concept of thermodynamics involving the capacity of hot bodies (more energetic subsystems) to produce work, thermodynamics is a theory of large-scale dynamical systems. As in thermodynamic systems, dynamical systems can exhibit energy that becomes unavailable to do useful work. This in turn contributes to an increase in system entropy; a measure of the tendency of a system to lose the ability to do useful work. In this section we use a large-scale

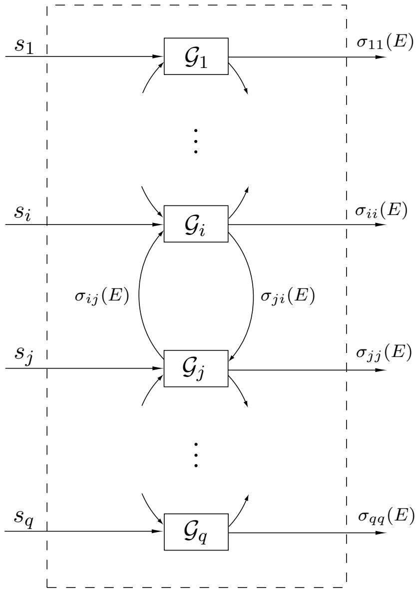

Fig. 1. Large-scale dynamical system $\mathcal{G}$

dynamical systems perspective to provide a system-theoretic foundation for thermodynamics.

To develop a system-theoretic foundation for thermodynamics, consider the large-scale dynamical system $\mathcal{G}$ shown in Figure 1 involving energy exchange between q interconnected subsystems. Let $v_{si} : \overline{\mathbb{R}}_+ \to \overline{\mathbb{R}}_+$ denote the energy (and hence a nonnegative quantity) of the ith subsystem, let $s_i : \overline{\mathbb{R}}_+ \to \mathbb{R}$ denote the external power (heat flux) supplied to (or extracted from) the ith subsystem, let $\sigma_{ij} : \overline{\mathbb{R}}_+^q \to \overline{\mathbb{R}}_+$, $i \neq j$, $i, j = 1, ..., q$, denote the instantaneous rate of energy (heat) flow from the jth subsystem to the ith subsystem, and let $\sigma_{ii} : \overline{\mathbb{R}}_+^q \to \overline{\mathbb{R}}_+^q$, $i = 1, ..., q$, denote the instantaneous rate of energy (heat) dissipation from the ith subsystem to the environment. Hence, an *energy balance* equation for the ith subsystem yields

$$\begin{aligned} v_{si}(T) &= v_{si}(t_0) \\ &\quad + \sum_{j=1,\, j\neq i}^{q} \int_{t_0}^{T} [\sigma_{ij}(V_s(t)) - \sigma_{ji}(V_s(t))]\mathrm{d}t \\ &\quad - \int_{t_0}^{T} \sigma_{ii}(V_s(t))\mathrm{d}t + \int_{t_0}^{T} s_i(t)\mathrm{d}t, \quad T \geq t_0, \end{aligned} \tag{2}$$

or, equivalently, in vector form,

$$\begin{aligned} V_s(T) &= V_s(t_0) + \int_{t_0}^{T} w(V_s(t))\mathrm{d}t - \int_{t_0}^{T} d(V_s(t))\mathrm{d}t \\ &\quad + \int_{t_0}^{T} S(t)\mathrm{d}t, \quad T \geq t_0, \end{aligned} \tag{3}$$

where $V_s(t) \triangleq [v_{s1}(t), ..., v_{sq}(t)]^{\mathrm{T}}$, $d(V_s(t)) \triangleq [\sigma_{11}(V_s(t)), ..., \sigma_{qq}(V_s(t))]^{\mathrm{T}}$, $S(t) \triangleq [s_1(t), ..., s_q(t)]^{\mathrm{T}}$, $t \geq t_0$, and $w = [w_1, ..., w_q]^{\mathrm{T}} : \overline{\mathbb{R}}_+^q \to \mathbb{R}^q$ is such that

$$w_i(V_s) = \sum_{j=1,\, j\neq i}^{q} [\sigma_{ij}(V_s) - \sigma_{ji}(V_s)], \quad V_s \in \overline{\mathbb{R}}_+^q. \tag{4}$$

Note that (2) yields a conservation of energy equation and implies that the energy stored in the ith subsystem is equal to the external energy supplied to (or extracted from) the ith subsystem plus the energy gained by the ith subsystem from all other subsystems due to subsystem coupling minus the energy dissipated from the ith subsystem to the environment. Equivalently, (2) can be rewritten as

$$\begin{aligned} \dot{v}_{si}(t) &= \sum_{j=1,\, j\neq i}^{q} [\sigma_{ij}(V_s(t)) - \sigma_{ji}(V_s(t))] - \sigma_{ii}(V_s(t)) \\ &\quad + s_i(t), \quad v_{si}(t_0) = v_{si0}, \quad t \geq t_0, \end{aligned} \tag{5}$$

or, in vector form,

$$\begin{aligned} \dot{V}_s(t) &= w(V_s(t)) - d(V_s(t)) + S(t),\ V_s(t_0) = V_{s0}, \\ &\qquad t \geq t_0, \end{aligned} \tag{6}$$

where $V_{s0} \triangleq [v_{s10}, ..., v_{sq0}]^{\mathrm{T}}$, yielding a *power balance* equation that characterizes energy flow between subsystems of the large-scale dynamical system $\mathcal{G}$. Equation (5) shows that the rate of change of energy, or power, in the ith subsystem is equal to the power input (heat flux) to the ith subsystem plus the energy (heat) flow to the ith subsystem from all other subsystems minus the power dissipated from the ith subsystem to the environment. Note that (3) or, equivalently, (6) is a statement of the *first law of thermodynamics* for each of the subsystems with $v_{si}(\cdot)$, $s_i(\cdot)$, $\sigma_{ij}(\cdot)$, $i \neq j$, and $\sigma_{ii}(\cdot)$, $i, j = 1, ..., q$, playing the role of the ith subsystem internal energy, rate of heat supplied to (or extracted from) the ith subsystem, heat flow between subsystems due to coupling, and the rate of energy (heat) dissipated to the environment, respectively. To further elucidate that (3) is essentially the statement of the principle of the conservation of energy let the total energy in the large-scale dynamical system $\mathcal{G}$ be given by $U \triangleq \mathbf{e}^{\mathrm{T}} V_s$, $V_s \in \overline{\mathbb{R}}_+^q$, where $\mathbf{e}^{\mathrm{T}} \triangleq [1, ..., 1]$, and let the energy received by the large-scale dynamical system $\mathcal{G}$ over the time interval $[t_1, t_2]$ be given by $Q \triangleq \int_{t_1}^{t_2} \mathbf{e}^{\mathrm{T}}[S(t) - d(V_s(t))]\mathrm{d}t$, where $V_s(t)$, $t \geq t_0$, is the solution to (6). Then, premultiplying (3) by $\mathbf{e}^{\mathrm{T}}$ and using the fact that $\mathbf{e}^{\mathrm{T}} w(V_s) \equiv 0$, it follows that

$$\Delta U = Q, \tag{7}$$

where $\Delta U \triangleq U(t_2) - U(t_1)$ denotes the variation in energy of the large-scale dynamical system $\mathcal{G}$ over the time interval $[t_1, t_2]$. This is a statement of the first law of thermodynamics for the large-scale dynamical system $\mathcal{G}$ and gives a precise formulation of the equivalence between variation in system internal energy and heat. It is important to note that our large-scale dynamical system model does not consider work done by the system on the environment nor work done by the environment on the system. Hence, Q can be interpreted physically as the amount of energy that is received by the system in forms other than work. The extension of addressing work performed by and on the system can be easily handeled by including an additional state equation, coupled to the power balance equation (6), involving volume states for each subsystem with exogenous pressure variables. Since this slight extension does not alter any of the results of the paper, it is not considered here for simplicity of exposition.

If the total energy of the large-scale dynamical system $\mathcal{G}$ at the initial and the final states is fixed, then it follows from (7) that the variation (δ) of the energy supplied to the large-scale dynamical system $\mathcal{G}$ is zero; that is, $\delta Q = 0$.

This implies that during a transformation between two fixed end points the large-scale dynamical system $\mathcal{G}$ receives a fixed amount of energy. In other words, for any two paths connecting the initial and final states of the dynamical system $\mathcal{G}$ the amount of energy supplied to the system is the same.

If $\sigma_{ij}(V_s) = 0$, $V_s \in \overline{\mathbb{R}}_+^q$, whenever $v_{sj} = 0$, $i,j = 1,...,q$, then $w(V_s) - d(V_s)$, $V_s \in \overline{\mathbb{R}}_+^q$, is essentially nonnegative. The above constraint implies that if the energy of the jth subsystem of $\mathcal{G}$ is zero, then this subsystem cannot supply any energy to its surroundings nor dissipate energy to the environment. Moreover, for the remainder of the paper we assume that $s_i(t) \geq 0$ whenever $v_{si}(t) = 0$, $t \geq t_0$, $i = 1,...,q$, which implies that when the energy of the ith subsystem is zero, then no energy can be extracted from this subsystem. The following proposition is needed for the main results of this paper.

Proposition 3.1: Consider the large-scale dynamical system $\mathcal{G}$ with power balance equation given by (6). Suppose $\sigma_{ij}(V_s) = 0$, $V_s \in \overline{\mathbb{R}}_+^q$, whenever $v_{sj} = 0$, $i,j = 1,...,q$, and $s_i(t) \geq 0$ whenever $v_{si}(t) = 0$, $t \geq t_0$, $i = 1,...,q$. Then the solution $V_s(t)$, $t \geq t_0$, to (6) is nonnegative for all nonnegative initial conditions $V_{s0} \in \overline{\mathbb{R}}_+^q$.

Proof. First note that $w(V_s) - d(V_s)$, $V_s \in \overline{\mathbb{R}}_+^q$, is essentially nonnegative. Next, since $s_i(t) \geq 0$ whenever $v_{si}(t) = 0$, $t \geq t_0$, $i = 1,...,q$, it follows that $\dot{v}_{si}(t) \geq 0$ for all $t \geq t_0$ and $i = 1,...,q$ whenever $v_{si}(t) = 0$ and $v_{sj}(t) \geq 0$ for all $j \neq i$ and $t \geq t_0$. This implies that for all nonnegative initial conditions $V_{s0} \in \overline{\mathbb{R}}_+^q$ the trajectory of $\mathcal{G}$ is directed towards the interior of the nonnegative orthant $\overline{\mathbb{R}}_+^q$ whenever $v_{si}(t) = 0$, $i = 1,...,q$, and hence remains nonnegative for all $t \geq t_0$. □

Next, premultiplying (3) by $\mathbf{e}^{\mathrm{T}}$, using Proposition 3.1, and using the fact that $\mathbf{e}^{\mathrm{T}} w(V_s) \equiv 0$, it follows that

$$\mathbf{e}^{\mathrm{T}} V_s(T) = \mathbf{e}^{\mathrm{T}} V_s(t_0) + \int_{t_0}^{T} \mathbf{e}^{\mathrm{T}} S(t)\mathrm{d}t - \int_{t_0}^{T} \mathbf{e}^{\mathrm{T}} d(V_s(t))\mathrm{d}t, \quad T \geq t_0. \quad (8)$$

Now, for the large-scale dynamical system $\mathcal{G}$ define the input $u(t) \triangleq S(t)$ and the output $y(t) \triangleq d(V_s(t))$. Hence, it follows from (8) that the large-scale dynamical system $\mathcal{G}$ is lossless [27] with respect to the *supply rate* $\mathbf{e}^{\mathrm{T}} u - \mathbf{e}^{\mathrm{T}} y$ and with the *storage function* $U(V_s) \triangleq \mathbf{e}^{\mathrm{T}} V_s$, $V_s \in \overline{\mathbb{R}}_+^q$. This implies that (see [27] for details)

$$0 \leq U_a(V_s) = U(V_s) = U_r(V_s) < \infty, \quad V_s \in \overline{\mathbb{R}}_+^q, \quad (9)$$

where

$$U_a(V_s) \triangleq - \inf_{u(\cdot),\, T \geq t_0} \int_{t_0}^{T} (\mathbf{e}^{\mathrm{T}} u(t) - \mathbf{e}^{\mathrm{T}} y(t))\mathrm{d}t, \quad (10)$$

$$U_r(V_s) \triangleq \inf_{u(\cdot),\, T \geq -t_0} \int_{-T}^{t_0} (\mathbf{e}^{\mathrm{T}} u(t) - \mathbf{e}^{\mathrm{T}} y(t))\mathrm{d}t. \quad (11)$$

Since $U_a(V_s)$ is the maximum amount of stored energy which can be extracted from the large-scale dynamical system $\mathcal{G}$ at any time T and $U_r(V_s)$ is the minimum amount of energy which can be delivered to the large-scale dynamical system $\mathcal{G}$ to transfer it from a state of minimum potential $V_s(-T) = 0$ to a given state $V_s(t_0) = V_{s0}$, it follows from (9) that the large-scale dynamical system $\mathcal{G}$ can deliver to its surroundings all of its stored subsystem energies and can store all of the work done to all of its subsystems. In the case where $S(t) \equiv 0$ it follows from (8) and the fact that $\sigma_{ii}(V_s) \geq 0$, $V_s \in \overline{\mathbb{R}}_+^q$, $i = 1,...,q$, that the zero solution $V_s(t) \equiv 0$ of the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) is Lyapunov stable with Lyapunov function $U(V_s)$ corresponding to the total energy in the system.

The nonlinear power balance equation (6) can exhibit a full range of nonlinear behavior including bifurcations, limit cycles, and even chaos. However, a thermodynamically consistent energy flow model should ensure that the evolution of the system energy is diffusive (parabolic) in character with convergent subsystem energies. Hence, to ensure a thermodynamically consistent energy flow model we require the following axioms. For the statement of these axioms we first recall the following graph theoretic notions.

Definition 3.1 ([37]): A *directed graph* $G(\mathcal{C})$ associated with the *connectivity matrix* $\mathcal{C} \in \mathbb{R}^{q\times q}$ has *vertices* $\{1, 2, ..., q\}$ and an *arc* from vertex i to vertex j, $i \neq j$, if and only if $\mathcal{C}_{(j,i)} \neq 0$. A *graph* $G(\mathcal{C})$ associated with the connectivity matrix $\mathcal{C} \in \mathbb{R}^{q\times q}$ is a directed graph for which the *arc set* is symmetric; that is, $\mathcal{C} = \mathcal{C}^{\mathrm{T}}$. We say that $G(\mathcal{C})$ is *strongly connected* if for any ordered pair of vertices (i,j), $i \neq j$, there exists a *path* (i.e., sequence of arcs) leading from i to j.

Recall that $\mathcal{C} \in \mathbb{R}^{q\times q}$ is *irreducible*; that is, there does not exist a permutation matrix such that $\mathcal{C}$ is cogredient to a lower block triangular matrix, if and only if $G(\mathcal{C})$ is strongly connected (see Theorem 2.7 of [37]). Let $\phi_{ij}(V_s) \triangleq \sigma_{ij}(V_s) - \sigma_{ji}(V_s)$, $V_s \in \overline{\mathbb{R}}_+^q$, define the net energy flow from the jth subsystem $\mathcal{G}_j$ to the ith subsystem $\mathcal{G}_i$ of the large-scale dynamical system $\mathcal{G}$. Axiom i): For the connectivity matrix $\mathcal{C} \in \mathbb{R}^{q\times q}$ associated with the large-scale dynamical system $\mathcal{G}$ defined by

$$\mathcal{C}_{(i,j)} = \begin{cases} 0, & \text{if } \phi_{ij}(V_s) \equiv 0, \\ 1, & \text{otherwise}, \end{cases} \quad i \neq j,\ i,j = 1,...,q, \quad (12)$$

and

$$\mathcal{C}_{(i,i)} = - \sum_{k=1,\, k\neq i}^{q} \mathcal{C}_{(k,i)}, \quad i = j, \quad i = 1,...,q, \quad (13)$$

rank $\mathcal{C} = q - 1$ and for $\mathcal{C}_{(i,j)} = 1$, $i \neq j$, $\phi_{ij}(V_s) = 0$ if and only if $v_{si} = v_{sj}$. Axiom ii): For $i,j = 1,...,q$, $(v_{si} - v_{sj})\phi_{ij}(V_s) \leq 0$, $V_s \in \overline{\mathbb{R}}_+^q$. The fact that $\phi_{ij}(V_s) = 0$ if and only if $v_{si} = v_{sj}$, $i \neq j$, implies that subsystems $\mathcal{G}_i$ and $\mathcal{G}_j$ of $\mathcal{G}$ are *connected*; alternatively, $\phi_{ij}(V_s) \equiv 0$ implies that $\mathcal{G}_i$ and $\mathcal{G}_j$ are *disconnected*. Axiom i) implies that if the energies in the connected subsystems $\mathcal{G}_i$ and $\mathcal{G}_j$ are equal, then energy exchange between these subsystems is not possible. This statement is consistent with the *zeroth law of thermodynamics* which postulates that temperature equality is a necessary and sufficient condition for thermal equilibrium. Furthermore, it follows from the fact that $\mathcal{C} = \mathcal{C}^{\mathrm{T}}$ and rank $\mathcal{C} = q - 1$ that the connectivity matrix $\mathcal{C}$ is irreducible which implies that for any pair of subsystems $\mathcal{G}_i$ and $\mathcal{G}_j$, $i \neq j$, of $\mathcal{G}$ there exists a sequence of connectors (arcs) of $\mathcal{G}$ that connect $\mathcal{G}_i$ and $\mathcal{G}_j$. Axiom ii) implies that energy flows from more energetic subsystems to less energetic subsystems and is consistent with the *second law* *of thermodynamics* which states that heat (energy) must flow in the direction of lower temperatures. Furthermore, note that $\phi_{ij}(V_{\rm s}) = -\phi_{ji}(V_{\rm s})$, $V_{\rm s} \in \overline{\mathbb{R}}^q_+$, $i \neq j$, $i,j = 1,...,q$, which implies conservation of energy between lossless subsystems. With $S(t) \equiv 0$, Axioms $i)$ and $ii)$ along with the fact that $\phi_{ij}(V_{\rm s}) = -\phi_{ji}(V_{\rm s})$, $V_{\rm s} \in \overline{\mathbb{R}}^q_+$, $i \neq j$, $i,j = 1,...,q$, imply that at a given instant of time energy can only be transported, stored, or dissipated but not created and the maximum amount of energy that can be transported and/or dissipated from a subsystem cannot exceed the energy in the subsystem.

Next, we establish that the classical Clausius inequality for reversible and irreversible thermodynamics is satisfied for our thermodynamically consistent energy flow model. For the remainder of the paper we assume that the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) is *reachable* from and *controllable* to the origin in $\overline{\mathbb{R}}^q_+$. Recall that the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) is reachable from the origin in $\overline{\mathbb{R}}^q_+$ if, for all $V_{\rm s0} = V_{\rm s}(t_0) \in \overline{\mathbb{R}}^q_+$, there exists a finite time $t_{\rm i} \leq t_0$ and a square integrable input $S(t)$ defined on $[t_{\rm i}, t_0]$ such that the state $V_{\rm s}(t)$, $t \geq t_{\rm i}$, can be driven from $V_{\rm s}(t_{\rm i}) = 0$ to $V_{\rm s}(t_0) = V_{\rm s0}$. Alternatively, $\mathcal{G}$ is controllable to the origin in $\overline{\mathbb{R}}^q_+$ if, for all $V_{\rm s0} = V_{\rm s}(t_0) \in \overline{\mathbb{R}}^q_+$, there exists a finite time $t_{\rm f} \geq t_0$ and a square integrable input $S(t)$ defined on $[t_0, t_{\rm f}]$ such that the state $V_{\rm s}(t)$, $t \geq t_0$, can be driven from $V_{\rm s}(t_0) = V_{\rm s0}$ to $V_{\rm s}(t_{\rm f}) = 0$. We let $\mathcal{U}_{\rm r} \subseteq \mathbb{R}^q$ denote the set of all admissible power inputs (heat flux) to the large-scale dynamical system $\mathcal{G}$ such that for any $T \geq -t_0$ the system energy state can be driven from $V_{\rm s}(-T) = 0$ to $V_{\rm s}(t_0) = V_{\rm s0} \in \overline{\mathbb{R}}^q_+$ by $S(\cdot) \in \mathcal{U}_{\rm r}$ and we let $\mathcal{U}_{\rm c} \subseteq \mathbb{R}^q$ denote the set of all admissible power inputs (heat flux) to the large-scale dynamical system $\mathcal{G}$ such that for any $T \geq t_0$ the system energy state can be driven from $V_{\rm s}(t_0) = V_{\rm s0} \in \overline{\mathbb{R}}^q_+$ to $V_{\rm s}(T) = 0$ by $S(\cdot) \in \mathcal{U}_{\rm c}$. For the next result $\oint$ denotes a cyclic integral evaluated along an arbitrary closed path of (6) in $\overline{\mathbb{R}}^q_+$, that is, $\oint \triangleq \int_{t_0}^{t_{\rm f}}$ with $t_{\rm f} \geq t_0$ and $S(\cdot) \in \mathbb{R}^q$ such that $V_{\rm s}(t_{\rm f}) = V_{\rm s}(t_0) = V_{\rm s0} \in \overline{\mathbb{R}}^q_+$.

Proposition 3.2: Consider the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) and assume that Axiom $ii)$ holds. Then for all $V_{\rm s0} \in \overline{\mathbb{R}}^q_+$, $t_{\rm f} \geq t_0$, and $S(t)$, $t \in [t_0, t_{\rm f}]$, such that $V_{\rm s}(t_{\rm f}) = V_{\rm s0}$,

$$\int_{t_0}^{t_{\rm f}} \sum_{i=1}^q \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t = \oint \sum_{i=1}^q \frac{{\rm d}Q_i(t)}{c + v_{{\rm s}i}(t)} \leq 0, \quad (14)$$

where $c > 0$, ${\rm d}Q_i(t) \triangleq [s_i(t) - \sigma_{ii}(V_{\rm s}(t))]{\rm d}t$, $i = 1,...,q$, is the amount of energy received by the ith subsystem over the infinitesimal time interval ${\rm d}t$, and $V_{\rm s}(t)$, $t \geq t_0$, is the solution to (6) with initial condition $V_{\rm s}(t_0) = V_{\rm s0}$.

Proof. Since, by Proposition 3.1, $V_{\rm s}(t) \geq\geq 0$, $t \geq t_0$, and $\phi_{ij}(V_{\rm s}) = -\phi_{ji}(V_{\rm s})$, $V_{\rm s} \in \overline{\mathbb{R}}^q_+$, $i \neq j$, $i,j = 1,...,q$, it follows from (6) and Axiom $ii)$ that

$$\begin{aligned}
\oint \sum_{i=1}^q \frac{{\rm d}Q_i(t)}{c + v_{{\rm s}i}(t)}
&= \int_{t_0}^{t_{\rm f}} \sum_{i=1}^q \frac{\dot{v}_{{\rm s}i}(t) - \sum_{j=1,\, j\neq i}^q \phi_{ij}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t \\
&= \sum_{i=1}^q \log_e \left(\frac{c + v_{{\rm s}i}(t_{\rm f})}{c + v_{{\rm s}i}(t_0)} \right) - \int_{t_0}^{t_{\rm f}} \sum_{i=1}^q \sum_{j=1,\, j\neq i}^q \frac{\phi_{ij}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t \\
&= -\int_{t_0}^{t_{\rm f}} \sum_{i=1}^q \sum_{j=i+1}^q \left(\frac{\phi_{ij}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} - \frac{\phi_{ij}(V_{\rm s}(t))}{c + v_{{\rm s}j}(t)} \right) {\rm d}t \\
&= -\int_{t_0}^{t_{\rm f}} \sum_{i=1}^q \sum_{j=i+1}^q \frac{\phi_{ij}(V_{\rm s}(t))[v_{{\rm s}j}(t) - v_{{\rm s}i}(t)]}{(c + v_{{\rm s}i}(t))(c + v_{{\rm s}j}(t))} {\rm d}t \\
&\leq 0, \qquad (15)
\end{aligned}$$

which proves the result. □

Inequality (14) is Clausius' inequality for reversible and irreversible thermodynamics as applied to large-scale dynamical systems. It follows from Axiom $i)$ and (6) that for the *isolated* large-scale dynamical system $\mathcal{G}$; that is, $S(t) \equiv 0$ and $d(V_{\rm s}(t)) \equiv 0$, the energy states given by $V_{\rm s\,e} = \alpha \mathbf{e}$, $\alpha \geq 0$, correspond to the equilibrium energy states of $\mathcal{G}$. Thus, as in classical thermodynamics, we can define a *reversible process* as a process where the trajectory of the large-scale dynamical system $\mathcal{G}$ moves along the set of equilibria of the isolated system $\mathcal{G}$. The power input that can generate such a trajectory can be given by $S(t) = d(V_{\rm s}(t)) + u(t)$, $t \geq t_0$, where $u(\cdot) \in \mathbb{R}^q$ is such that $u_i(t) \equiv u_j(t)$, $i \neq j$, $i,j = 1,...,q$. Alternatively, an *irreversible process* is a process that is not reversible. Hence, it follows from Axiom $i)$ that for a reversible process $\phi_{ij}(V_{\rm s}(t)) \equiv 0$, $t \geq t_0$, $i \neq j$, $i,j = 1,...,q$, and thus, by Proposition 3.2, inequality (14) is satisfied as an equality. Alternatively, for an irreversible process it follows from Axioms $i)$ and $ii)$ that (14) is satisfied as a strict inequality.

Next, we give a deterministic definition of entropy for the large-scale dynamical system $\mathcal{G}$ that is consistent with the classical thermodynamic definition of entropy.

Definition 3.2: For the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6), a function $\mathcal{S} : \overline{\mathbb{R}}^q_+ \to \mathbb{R}$ satisfying

$$\mathcal{S}(V_{\rm s}(t_2)) \geq \mathcal{S}(V_{\rm s}(t_1)) + \int_{t_1}^{t_2} \sum_{i=1}^q \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t, \quad (16)$$

for any $t_2 \geq t_1 \geq t_0$ and $S(t)$, $t \in [t_1, t_2]$, is called the *entropy* of $\mathcal{G}$.

Next, we show that (14) guarantees the existence of an entropy function for $\mathcal{G}$. For this result define

$$\mathcal{S}_{\rm a}(V_{\rm s0}) \triangleq -\sup_{S(\cdot) \in \mathcal{U}_{\rm c},\, T \geq t_0} \int_{t_0}^{T} \sum_{i=1}^q \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t, \quad (17)$$

where $V_{\rm s}(t_0) = V_{\rm s0} \in \overline{\mathbb{R}}^q_+$ and $V_{\rm s}(T) = 0$, and define

$$\mathcal{S}_{\rm r}(V_{\rm s0}) \triangleq \sup_{S(\cdot) \in \mathcal{U}_{\rm r},\, T \geq -t_0} \int_{-T}^{t_0} \sum_{i=1}^q \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t, \quad (18)$$

where $V_{\rm s}(-T) = 0$ and $V_{\rm s}(t_0) = V_{\rm s0} \in \overline{\mathbb{R}}^q_+$.

Theorem 3.1: Consider the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) and assume that Axiom $ii)$ holds. Then there exists an entropy function for $\mathcal{G}$. Moreover, $\mathcal{S}_{\rm a}(V_{\rm s})$, $V_{\rm s} \in \overline{\mathbb{R}}_+^q$, and $\mathcal{S}_{\rm r}(V_{\rm s})$, $V_{\rm s} \in \overline{\mathbb{R}}_+^q$, are possible entropy functions for $\mathcal{G}$ with $\mathcal{S}_{\rm a}(0) = \mathcal{S}_{\rm r}(0) = 0$. Finally, all entropy functions $\mathcal{S}(V_{\rm s})$, $V_{\rm s} \in \overline{\mathbb{R}}_+^q$, for $\mathcal{G}$ satisfy

$$\mathcal{S}_{\rm r}(V_{\rm s}) \le \mathcal{S}(V_{\rm s}) - \mathcal{S}(0) \le \mathcal{S}_{\rm a}(V_{\rm s}), \quad V_{\rm s} \in \overline{\mathbb{R}}_+^q. \tag{19}$$

Proof. Since $\mathcal{G}$ is controllable to and reachable from the origin in $\overline{\mathbb{R}}_+^q$ it follows from (17) and (18) that $\mathcal{S}_{\rm a}(V_{\rm s0}) < \infty$, $V_{\rm s0} \in \overline{\mathbb{R}}_+^q$, and $\mathcal{S}_{\rm r}(V_{\rm s0}) > -\infty$, $V_{\rm s0} \in \overline{\mathbb{R}}_+^q$, respectively. Next, let $V_{\rm s0} \in \overline{\mathbb{R}}_+^q$ and let $S(t)$, $t \in [t_{\rm i}, t_{\rm f}]$, where $t_{\rm i} \le t_0 \le t_{\rm f}$, be such that $V_{\rm s}(t_{\rm i}) = V_{\rm s}(t_{\rm f}) = 0$ and $V_{\rm s}(t_0) = V_{\rm s0}$. In this case, it follows from (14) that

$$\int_{t_{\rm i}}^{t_{\rm f}} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t \le 0, \tag{20}$$

or, equivalently,

$$\int_{t_{\rm i}}^{t_0} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t \le -\int_{t_0}^{t_{\rm f}} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t. \tag{21}$$

Now, taking the supremum on both sides of (21) over all $S(\cdot) \in \mathcal{U}_{\rm r}$ and $t_{\rm i} \le t_0$ yields

$$\begin{aligned} \mathcal{S}_{\rm r}(V_{\rm s0}) &= \sup_{S(\cdot)\in\mathcal{U}_{\rm r},\, t_{\rm i}\le t_0} \int_{t_{\rm i}}^{t_0} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t \\ &\le -\int_{t_0}^{t_{\rm f}} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t. \end{aligned} \tag{22}$$

Next, taking the infimum on both sides of (22) over all $S(\cdot) \in \mathcal{U}_{\rm c}$ and $t_{\rm f} \ge t_0$ we obtain $S_{\rm r}(V_{\rm s0}) \le \mathcal{S}_{\rm a}(V_{\rm s0})$, $V_{\rm s0} \in \overline{\mathbb{R}}_+^q$, which implies that $-\infty < S_{\rm r}(V_{\rm s0}) \le \mathcal{S}_{\rm a}(V_{\rm s0}) < \infty$, $V_{\rm s0} \in \overline{\mathbb{R}}_+^q$. Hence, the functions $\mathcal{S}_{\rm a}(\cdot)$ and $\mathcal{S}_{\rm r}(\cdot)$ are well defined. Next, it follows from the definition of $\mathcal{S}_{\rm a}(\cdot)$ that, for any $T \ge t_1$ and $S(\cdot) \in \mathcal{U}_{\rm c}$ such that $V_{\rm s}(t_1) \in \overline{\mathbb{R}}_+^q$ and $V_{\rm s}(T) = 0$,

$$\begin{aligned} -\mathcal{S}_{\rm a}(V_{\rm s}(t_1)) \ &\ge \ \int_{t_1}^{t_2} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t \\ &\quad + \int_{t_2}^{T} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t, \quad t_1 \le t_2 \le T, \end{aligned} \tag{23}$$

and hence

$$\begin{aligned} -\mathcal{S}_{\rm a}(V_{\rm s}(t_1)) \ &\ge \ \int_{t_1}^{t_2} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t \\ &\quad + \sup_{S(\cdot)\in\mathcal{U}_{\rm c},\, T\ge t_2} \int_{t_2}^{T} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t \\ &= \int_{t_1}^{t_2} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t - \mathcal{S}_{\rm a}(V_{\rm s}(t_2)), \end{aligned} \tag{24}$$

which implies that $\mathcal{S}_{\rm a}(V_{\rm s})$, $V_{\rm s} \in \overline{\mathbb{R}}_+^q$, satisfies (16). Thus, $\mathcal{S}_{\rm a}(V_{\rm s})$, $V_{\rm s} \in \overline{\mathbb{R}}_+^q$, is a possible entropy function for $\mathcal{G}$. Note that with $V_{\rm s}(t_0) = V_{\rm s}(T) = 0$ it follows from (14) that supremum in (17) is taken over the set of nonpositive values with one of the values being zero for $S(t) \equiv 0$. Thus, $\mathcal{S}_{\rm a}(0) = 0$. Similarly, it can be shown that $\mathcal{S}_{\rm r}(V_{\rm s})$, $V_{\rm s} \in \overline{\mathbb{R}}_+^q$, given by (18) satisfies (16) and hence is a possible entropy function for the system $\mathcal{G}$ with $\mathcal{S}_{\rm r}(0) = 0$.

Next, suppose there exists an entropy function $\mathcal{S} : \overline{\mathbb{R}}_+^q \to \mathbb{R}$ for $\mathcal{G}$ and let $V_{\rm s}(t_2) = 0$ in (16). Then it follows from (16) that

$$\mathcal{S}(V_{\rm s}(t_1)) - \mathcal{S}(0) \le -\int_{t_1}^{t_2} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t, \tag{25}$$

for all $t_2 \ge t_1$ and $S(\cdot) \in \mathcal{U}_{\rm c}$ which implies that

$$\begin{aligned} \mathcal{S}(V_{\rm s}(t_1)) \ - \ \mathcal{S}(0) & \\ &\le \inf_{S(\cdot)\in\mathcal{U}_{\rm c},\, t_2\ge t_1} \left[-\int_{t_1}^{t_2} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t \right] \\ &= -\sup_{S(\cdot)\in\mathcal{U}_{\rm c},\, t_2\ge t_1} \int_{t_1}^{t_2} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t \\ &= \mathcal{S}_{\rm a}(V_{\rm s}(t_1)). \end{aligned} \tag{26}$$

Since $V_{\rm s}(t_1)$ is arbitrary, it follows that $\mathcal{S}(V_{\rm s}) - \mathcal{S}(0) \le \mathcal{S}_{\rm a}(V_{\rm s})$, $V_{\rm s} \in \overline{\mathbb{R}}_+^q$. Alternatively, let $V_{\rm s}(t_1) = 0$ in (16). Then it follows from (16) that

$$\mathcal{S}(V_{\rm s}(t_2)) - \mathcal{S}(0) \ge \int_{t_1}^{t_2} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t, \tag{27}$$

for all $t_1 \le t_2$ and $S(\cdot) \in \mathcal{U}_{\rm r}$. Hence,

$$\begin{aligned} \mathcal{S}(V_{\rm s}(t_2)) \ - \ \mathcal{S}(0) & \\ &\ge \sup_{S(\cdot)\in\mathcal{U}_{\rm r},\, t_1\le t_2} \int_{t_1}^{t_2} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} {\rm d}t \\ &= \mathcal{S}_{\rm r}(V_{\rm s}(t_2)), \end{aligned} \tag{28}$$

which, since $V_{\rm s}(t_2)$ is arbitrary, implies that $\mathcal{S}_{\rm r}(V_{\rm s}) \le \mathcal{S}(V_{\rm s}) - \mathcal{S}(0)$, $V_{\rm s} \in \overline{\mathbb{R}}_+^q$. Thus, all entropy functions for $\mathcal{G}$ satisfy (19). $\square$

Remark 3.1: It is important to note that inequality (14) is equivalent to the existence of an entropy function for $\mathcal{G}$. Sufficiency is simply a statement of Theorem 3.1 while necessity follows from (16) with $V_{\rm s}(t_2) = V_{\rm s}(t_1)$. For irreversible thermodynamics with power balance equation (6), Definition 3.2 does not provide enough information to define the entropy uniquely. This difficulty has long been pointed out in [39]. For reversible thermodynamics this ambiguity is not an issue as (14) holds as an equality for a reversible process since $\phi_{ij}(V_{\rm s}(t)) \equiv 0$, $i \ne j$, $i,j = 1,...,q$, and in this case it can be shown that $\mathcal{S}_{\rm a}(V_{\rm s}) = \mathcal{S}_{\rm r}(V_{\rm s}) = \mathcal{S}(V_{\rm s}) - \mathcal{S}(0) = \mathbf{e}^{\rm T}\mathbf{log}_e(c\mathbf{e} + V_{\rm s}) - q\log_e c$, where $V_{\rm s} = V_{\rm s\,e}$ and $\mathbf{log}_e(c\mathbf{e} + V_{\rm s})$ denotes the vector natural logarithm given by $[\log_e(c+v_{\rm s1}), ..., \log_e(c+v_{{\rm s}q})]^{\rm T}$. This definition of entropy leads to the second law of thermodynamics being viewed as an axiom in the context of (anti)cyclo-dissipative dynamical systems [27], [40]. A similar remark holds for the definition of ectropy introduced below.

The next result shows that all entropy functions for $\mathcal{G}$ are continuous on $\overline{\mathbb{R}}_+^q$. First, however, the following lemma is required.

Lemma 3.1: Consider the large-scale dynamical system $\mathcal{G}$ with power balance equation (6). Then for every equilibrium state $E_{\rm e} \in \overline{\mathbb{R}}_+^q$ and every $\varepsilon > 0$ and $T > 0$, there exists $S_{\rm e} \in \mathbb{R}^q$, $\alpha > 0$, and $\hat{T} \in [0, T]$ such that for every $\hat{E} \in \overline{\mathbb{R}}_+^q$ with $\|\hat{E} - E_{\rm e}\| \leq \alpha T$, there exists $S : [0, \hat{T}] \to \mathbb{R}^q$ such that $\|S(t) - S_{\rm e}\| \leq \varepsilon$, $t \in [0, \hat{T}]$, and $E(t) = E_{\rm e} + \frac{(\hat{E} - E_{\rm e})}{\hat{T}} t$, $t \in [0, \hat{T}]$.

Proof. Note that with $S_{\rm e} = d(E_{\rm e}) - w(E_{\rm e})$, the state $E_{\rm e} \in \overline{\mathbb{R}}_+^q$ is an equilibrium state of (6). Let $\theta > 0$ and $T > 0$ and define

$$M(\theta, T) \triangleq \max_{E \in \mathcal{B}_1(0), t \in [0,T]} \|w(E_{\rm e} + \theta t E) - d(E_{\rm e} + \theta t E) + S_{\rm e}\|. \tag{29}$$

Note that for every $T > 0$, $\lim_{\theta \to 0^+} M(\theta, T) = 0$ and for every $\theta > 0$, $\lim_{T \to 0^+} M(\theta, T) = 0$. Next, let $\varepsilon > 0$ and $T > 0$ be given and let $\alpha > 0$ be such that $M(\alpha, T) + \alpha \leq \varepsilon$. (Note that $\alpha \leq \varepsilon$; the existence of such an α is guaranteed since $M(\alpha, T) \to 0$ as $\alpha \to 0^+$.) Now, let $\hat{E} \in \overline{\mathbb{R}}_+^q$ be such that $\|\hat{E} - E_{\rm e}\| \leq \alpha T$. With $\hat{T} \triangleq \frac{\|\hat{E} - E_{\rm e}\|}{\alpha} \leq T$ and

$$S(t) = -w(E(t)) + d(E(t)) + \alpha \frac{(\hat{E} - E_{\rm e})}{\|\hat{E} - E_{\rm e}\|},\ t \in [0, \hat{T}],$$

it follows that

$$E(t) = E_{\rm e} + \frac{(\hat{E} - E_{\rm e})}{\|\hat{E} - E_{\rm e}\|} \alpha t, \quad t \in [0, \hat{T}], \tag{30}$$

is a solution to (6). The result is now immediate by noting that $E(\hat{T}) = \hat{E}$ and

$$\begin{aligned} \|S(t) - S_{\rm e}\| &\leq \|w\left(E_{\rm e} + \tfrac{(\hat{E} - E_{\rm e})}{\|\hat{E} - E_{\rm e}\|} \alpha t\right) \\ &\quad - d\left(E_{\rm e} + \tfrac{(\hat{E} - E_{\rm e})}{\|\hat{E} - E_{\rm e}\|} \alpha t\right) + S_{\rm e}\| + \alpha \\ &\leq M(\alpha, T) + \alpha \leq \varepsilon, \quad t \in [0, \hat{T}]. \end{aligned} \tag{31}$$

□

Theorem 3.2: Consider the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) and let $\mathcal{S} : \overline{\mathbb{R}}_+^q \to \mathbb{R}$ be an entropy function of $\mathcal{G}$. Then $\mathcal{S}(\cdot)$ is continuous on $\overline{\mathbb{R}}_+^q$.

Proof. Let $E_{\rm e} \in \overline{\mathbb{R}}_+^q$ and $S_{\rm e} \in \mathbb{R}^q$ be such that $s_{{\rm e}i} = \sigma_{ii}(E_{\rm e}) - \sum_{j=1, j \neq i}^q \phi_{ij}(E_{\rm e})$, $i = 1, \ldots, q$. Note that with $S(t) \equiv S_{\rm e}$, $E_{\rm e}$ is an equilibrium point of the power balance equation (6). Next, it follows from Lemma 3.1 that $\mathcal{G}$ is locally controllable; that is, for every $T > 0$ and $\varepsilon > 0$ the set of points which can be reached from and to $E_{\rm e}$ in time T using admissible inputs $S : [0, T] \to \mathbb{R}^q$, satisfying $\|S(t) - S_{\rm e}\| < \varepsilon$, contains a neighborhood of $E_{\rm e}$. Next, let $\delta > 0$ and note that it follows from the continuity of $w(\cdot)$ and $d(\cdot)$ that there exist $T > 0$ and $\varepsilon > 0$ such that for every $S : [0, T) \to \mathbb{R}^q$ and $\|S(t) - S_{\rm e}\| < \varepsilon$, $\|E(t) - E_{\rm e}\| < \delta$, $t \in [0, T)$, where $E(t)$, $t \in [0, T)$, denotes the solution to (6) with the initial condition $E_{\rm e}$. Furthermore, it follows from the local controllability of $\mathcal{G}$ that for every $\hat{T} \in (0, T]$ there exists a strictly increasing, continuous function $\gamma : \mathbb{R} \to \mathbb{R}$ such that $\gamma(0) = 0$ and for every $E_0 \in \overline{\mathbb{R}}_+^q$ such that $\|E_0 - E_{\rm e}\| \leq \gamma(\hat{T})$, there exists $\hat{t} \in [0, \hat{T}]$ and an input $S : [0, \hat{T}] \to \mathbb{R}^q$ such that $\|S(t) - S_{\rm e}\| < \varepsilon$, $t \in [0, \hat{t})$, and $E(\hat{t}) = E_0$. In addition, it follows from Lemma 3.1 that $S : [0, \hat{T}] \to \mathbb{R}^q$ is such that $E(t) \geq\geq 0$, $t \in [0, \hat{T}]$. Next, since $\sigma_{ii}(\cdot)$, $i = 1, \ldots, q$, is continuous it follows that there exists $M \in (0, \infty)$ such that

$$\sup_{\|E - E_{\rm e}\| < \delta,\ \|S - S_{\rm e}\| < \varepsilon} \sum_{i=1}^q \frac{s_i - \sigma_{ii}(E)}{c + e_i} = M. \tag{32}$$

Hence, it follows that

$$\begin{aligned} &\left| \int_0^{\hat{t}} \sum_{i=1}^q \frac{s_i(\sigma) - \sigma_{ii}(E(\sigma))}{c + e_i(\sigma)} {\rm d}\sigma \right| \\ &\qquad \leq \int_0^{\hat{t}} \left| \sum_{i=1}^q \frac{s_i(\sigma) - \sigma_{ii}(E(\sigma))}{c + e_i(\sigma)} \right| {\rm d}\sigma \\ &\qquad \leq M\hat{t} \leq M\hat{T} \leq \gamma^{-1}(\|E_0 - E_{\rm e}\|). \end{aligned} \tag{33}$$

Now, if $\mathcal{S}(\cdot)$ is an entropy function of $\mathcal{G}$, then

$$\mathcal{S}(E(\hat{t})) \geq \mathcal{S}(E_{\rm e}) + \int_0^{\hat{t}} \sum_{i=1}^q \frac{s_i(\sigma) - \sigma_{ii}(E(\sigma))}{c + e_i(\sigma)} {\rm d}\sigma, \tag{34}$$

or, equivalently,

$$-\int_0^{\hat{t}} \sum_{i=1}^q \frac{s_i(\sigma) - \sigma_{ii}(E(\sigma))}{c + e_i(\sigma)} {\rm d}\sigma \geq \mathcal{S}(E_{\rm e}) - \mathcal{S}(E(\hat{t})). \tag{35}$$

If $\mathcal{S}(E_{\rm e}) \geq \mathcal{S}(E(\hat{t}))$, then combining (33) and (35) yields

$$|\mathcal{S}(E_{\rm e}) - \mathcal{S}(E(\hat{t}))| \leq \gamma^{-1}(\|E_0 - E_{\rm e}\|). \tag{36}$$

Alternatively, if $\mathcal{S}(E(\hat{t})) \geq \mathcal{S}(E_{\rm e})$, then (36) can be derived by reversing the roles of $\hat{E}$ and $E(\hat{t})$. In particular, using the fact that $\mathcal{G}$ is locally controllable from and to $E_{\rm e}$, similar arguments can be used to show that the set of points which can be steered in small time to $E_{\rm e}$ contains a neighborhood of $E(\hat{t})$. Hence, since $\gamma(\cdot)$ is continuous and $E(\hat{t})$ is arbitrary, it follows that $\mathcal{S}(\cdot)$ is continuous on $\overline{\mathbb{R}}_+^q$.

□

The next proposition shows that if (16) holds as an equality for some transformation starting and ending at an equilibrium point of the isolated system $\mathcal{G}$, then this transformation must be reversible.

Proposition 3.3: Consider the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) and assume that Axioms $i)$ and $ii)$ hold. Let $\mathcal{S}(\cdot)$ denote an entropy of $\mathcal{G}$ and let $E : [t_0, t_1] \to \overline{\mathbb{R}}_+^q$ denote the solution to (6) with $E(t_0) = \alpha_0 \mathbf{e}$ and $E(t_1) = \alpha_1 \mathbf{e}$, where α_0, $\alpha_1 \geq 0$. Then,

$$\mathcal{S}(E(t_1)) = \mathcal{S}(E(t_0)) + \int_{t_0}^{t_1} \sum_{i=1}^q \frac{s_i(t) - \sigma_{ii}(E(t))}{c + e_i(t)} {\rm d}t \tag{37}$$

if and only if there exists $\alpha : [t_0, t_1] \to \overline{\mathbb{R}}_+$ such that $\alpha(t_0) = \alpha_0$, $\alpha(t_1) = \alpha_1$, and $E(t) = \alpha(t)\mathbf{e}$, $t \in [t_0, t_1]$.

Proof. Since $E(t_0)$ and $E(t_1)$ are equilibrium states of the isolated system $\mathcal{G}$ it follows from Remark 3.1 that

$$\begin{aligned} \mathcal{S}(E(t_1)) - \mathcal{S}(E(t_0)) &= q \log_e(c + \alpha_1) \\ &\quad - q \log_e(c + \alpha_0). \end{aligned} \tag{38}$$

Furthermore, it follows from (6) that

$$\begin{aligned}\int_{t_0}^{t_1}\sum_{i=1}^{q}\frac{s_i(t)-\sigma_{ii}(E(t))}{c+e_i(t)}\mathrm{d}t\\ =\int_{t_0}^{t_1}\sum_{i=1}^{q}\frac{\dot{e}_i(t)-\sum_{j=1,j\neq i}^{q}\phi_{ij}(E(t))}{c+e_i(t)}\mathrm{d}t\\ =q\log_e\left(\frac{c+\alpha_1}{c+\alpha_0}\right)\\ -\int_{t_0}^{t_1}\sum_{i=1}^{q}\sum_{j=i+1}^{q}\frac{\phi_{ij}(E(t))(e_j(t)-e_i(t))}{(c+e_i(t))(c+e_j(t))}\mathrm{d}t.\end{aligned}\quad (39)$$

Now, it follows from Axioms $i)$ and $ii)$ that (37) holds if and only if $e_i(t)=e_j(t)$, $t\in[t_0,t_1]$, $i\neq j$, $i,j=1,...,q$, or equivalently, there exists $\alpha:[t_0,t_1]\to\overline{\mathbb{R}}_+$ such that $E(t)=\alpha(t)\mathbf{e}$, $t\in[t_0,t_1]$. □

The next proposition gives a closed-form expression for the entropy of $\mathcal{G}$.

Proposition 3.4: Consider the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) and assume that Axiom $ii)$ holds. Then the function $\mathcal{S}:\overline{\mathbb{R}}_+^q\to\mathbb{R}$ given by

$$\mathcal{S}(V_{\mathrm{s}})=\mathbf{e}^{\mathrm{T}}\mathbf{log}_e(c\mathbf{e}+V_{\mathrm{s}})-q\log_e c,\quad V_{\mathrm{s}}\in\overline{\mathbb{R}}_+^q,\quad (40)$$

where $c>0$, is an entropy function of $\mathcal{G}$.

Proof. Since, by Proposition 3.1, $V_{\mathrm{s}}(t)\geq\geq 0$, $t\geq t_0$, and $\phi_{ij}(V_{\mathrm{s}})=-\phi_{ji}(V_{\mathrm{s}})$, $V_{\mathrm{s}}\in\overline{\mathbb{R}}_+^q$, $i\neq j$, $i,j=1,...,q$, it follows that

$$\begin{aligned}\dot{\mathcal{S}}(V_{\mathrm{s}}(t)) &= \sum_{i=1}^{q}\frac{\dot{v}_{\mathrm{s}i}(t)}{c+v_{\mathrm{s}i}(t)}\\ &= \sum_{i=1}^{q}\frac{s_i(t)-\sigma_{ii}(V_{\mathrm{s}}(t))}{c+v_{\mathrm{s}i}(t)}+\sum_{i=1}^{q}\sum_{j=1,\,j\neq i}^{q}\frac{\phi_{ij}(V_{\mathrm{s}}(t))}{c+v_{\mathrm{s}i}(t)}\\ &= \sum_{i=1}^{q}\frac{s_i(t)-\sigma_{ii}(V_{\mathrm{s}}(t))}{c+v_{\mathrm{s}i}(t)}+\sum_{i=1}^{q}\sum_{j=i+1}^{q}\left(\frac{\phi_{ij}(V_{\mathrm{s}}(t))}{c+v_{\mathrm{s}i}(t)}-\frac{\phi_{ij}(V_{\mathrm{s}}(t))}{c+v_{\mathrm{s}j}(t)}\right)\\ &= \sum_{i=1}^{q}\frac{s_i(t)-\sigma_{ii}(V_{\mathrm{s}}(t))}{c+v_{\mathrm{s}i}(t)}+\sum_{i=1}^{q}\sum_{j=i+1}^{q}\frac{\phi_{ij}(V_{\mathrm{s}}(t))(v_{\mathrm{s}j}(t)-v_{\mathrm{s}i}(t))}{(c+v_{\mathrm{s}i}(t))(c+v_{\mathrm{s}j}(t))}\\ &\geq \sum_{i=1}^{q}\frac{s_i(t)-\sigma_{ii}(V_{\mathrm{s}}(t))}{c+v_{\mathrm{s}i}(t)},\quad t\geq t_0.\end{aligned}\quad (41)$$

Now, integrating (41) over $[t_1,\,t_2]$ yields (16). □

Remark 3.2: Note that it follows from the last equality in (41) that the entropy function given by (40) satisfies (16) as an equality for a reversible process and as a strict inequality for an irreversible process.

The entropy expression given by (40) is identical in form to the Boltzmann entropy for statistical thermodynamics. Due to the fact that the entropy is indeterminate to the extent of an additive constant, we can place the constant of integration $q\log_e c$ to zero by taking $c=1$. Since $\mathcal{S}(V_{\mathrm{s}})$ given by (40) achieves a maximum when all the subsystem energies $v_{\mathrm{s}i}$, $i=1,...,q$, are equal, entropy can be thought of as a measure of the tendency of a system to lose the ability to do useful work and lose order and to settle to a more homogenous state.

Recalling that $\mathrm{d}Q_i(t)=[s_i(t)-\sigma_{ii}(V_{\mathrm{s}}(t))]\mathrm{d}t$, $i=1,...,q$, is the infinitesimal amount of heat received or dissipated by the ith subsystem of $\mathcal{G}$ over the infinitesimal time interval $\mathrm{d}t$, it follows from (16) that

$$\mathrm{d}\mathcal{S}(V_{\mathrm{s}}(t))\geq\sum_{i=1}^{q}\frac{\mathrm{d}Q_i(t)}{c+v_{\mathrm{s}i}(t)},\quad t\geq t_0.\quad (42)$$

Inequality (42) is analogous to the classical thermodynamic inequality for the variation of entropy during an infinitesimal irreversible transformation with the shifted subsystem energies $c+v_{\mathrm{s}i}$ playing the role of the ith subsystem thermodynamic (absolute) temperatures.

Next, we introduce a *new* and dual notion to entropy; namely ectropy, describing the status quo of the large-scale dynamical system $\mathcal{G}$. First, however, we present a dual to inequality (14) that holds for our thermodynamically consistent energy flow model.

Proposition 3.5: Consider the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) and assume that Axiom $ii)$ holds. Then for all $V_{\mathrm{s}0}\in\overline{\mathbb{R}}_+^q$, $t_{\mathrm{f}}\geq t_0$, and $S(t)$, $t\in[t_0,t_{\mathrm{f}}]$, such that $V_{\mathrm{s}}(t_{\mathrm{f}})=V_{\mathrm{s}0}$,

$$\begin{aligned}\int_{t_0}^{t_{\mathrm{f}}}\sum_{i=1}^{q}v_{\mathrm{s}i}(t)[s_i(t)-\sigma_{ii}(V_{\mathrm{s}}(t))]\mathrm{d}t\\ =\oint\sum_{i=1}^{q}v_{\mathrm{s}i}(t)\mathrm{d}Q_i(t)\geq 0,\end{aligned}\quad (43)$$

where $V_{\mathrm{s}}(t)$, $t\geq t_0$, is the solution to (6) with initial condition $V_{\mathrm{s}}(t_0)=V_{\mathrm{s}0}$.

Proof. Since, by Proposition 3.1, $V_{\mathrm{s}}(t)\geq\geq 0$, $t\geq t_0$, and $\phi_{ij}(V_{\mathrm{s}})=-\phi_{ji}(V_{\mathrm{s}})$, $V_{\mathrm{s}}\in\overline{\mathbb{R}}_+^q$, $i\neq j$, $i,j=1,...,q$, it follows from (6) and Axiom $ii)$ that

$$\begin{aligned}\oint\sum_{i=1}^{q}v_{\mathrm{s}i}(t)\mathrm{d}Q_i(t)\\ =\int_{t_0}^{t_{\mathrm{f}}}\sum_{i=1}^{q}v_{\mathrm{s}i}(t)[\dot{v}_{\mathrm{s}i}(t)-\sum_{j=1,\,j\neq i}^{q}\phi_{ij}(V_{\mathrm{s}}(t))]\mathrm{d}t\\ =\tfrac{1}{2}V_{\mathrm{s}}^{\mathrm{T}}(t_{\mathrm{f}})V_{\mathrm{s}}(t_{\mathrm{f}})-\tfrac{1}{2}V_{\mathrm{s}}^{\mathrm{T}}(t_0)V_{\mathrm{s}}(t_0)\\ -\int_{t_0}^{t_{\mathrm{f}}}\sum_{i=1}^{q}\sum_{j=1,\,j\neq i}^{q}v_{\mathrm{s}i}(t)\phi_{ij}(V_{\mathrm{s}}(t))\mathrm{d}t\\ =-\int_{t_0}^{t_{\mathrm{f}}}\sum_{i=1}^{q}\sum_{j=i+1}^{q}\phi_{ij}(V_{\mathrm{s}}(t))[v_{\mathrm{s}i}(t)-v_{\mathrm{s}j}(t)]\mathrm{d}t\\ \geq 0,\end{aligned}\quad (44)$$

which proves the result. □

Note that inequality (43) is satisfied as an equality for a reversible process and as a strict inequality for an irreversible process. Next, we present definition of ectropy for the large-scale dynamical system $\mathcal{G}$.

Definition 3.3: For the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6), a function $\mathcal{E}:\overline{\mathbb{R}}_+^q\to\mathbb{R}$ satisfying

$$\mathcal{E}(V_{\rm s}(t_2)) \le \mathcal{E}(V_{\rm s}(t_1)) + \int_{t_1}^{t_2}\sum_{i=1}^{q} v_{{\rm s}i}(t)[s_i(t)-\sigma_{ii}(V_{\rm s}(t))]{\rm d}t, \quad (45)$$

for any $t_2 \ge t_1 \ge t_0$ and $S(t)$, $t\in[t_1,t_2]$, is called the *ectropy* of $\mathcal{G}$.

For the next result define

$$\mathcal{E}_{\rm a}(V_{\rm s0}) \triangleq -\inf_{S(\cdot)\in\mathcal{U}_{\rm c},\, T\ge t_0}\int_{t_0}^{T}\sum_{i=1}^{q} v_{{\rm s}i}(t)[s_i(t)-\sigma_{ii}(V_{\rm s}(t))]{\rm d}t, \quad (46)$$

where $V_{\rm s}(t_0)=V_{\rm s0}\in\overline{\mathbb{R}}_+^q$ and $V_{\rm s}(T)=0$, and

$$\mathcal{E}_{\rm r}(V_{\rm s0}) \triangleq \inf_{S(\cdot)\in\mathcal{U}_{\rm r},\, T\ge -t_0}\int_{-T}^{t_0}\sum_{i=1}^{q} v_{{\rm s}i}(t)[s_i(t)-\sigma_{ii}(V_{\rm s}(t))]{\rm d}t, \quad (47)$$

where $V_{\rm s}(-T)=0$ and $V_{\rm s}(t_0)=V_{\rm s0}\in\overline{\mathbb{R}}_+^q$.

Theorem 3.3: Consider the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) and assume that Axiom $ii)$ holds. Then there exists an ectropy function for $\mathcal{G}$. Moreover, $\mathcal{E}_{\rm a}(V_{\rm s})$, $V_{\rm s}\in\overline{\mathbb{R}}_+^q$, and $\mathcal{E}_{\rm r}(V_{\rm s})$, $V_{\rm s}\in\overline{\mathbb{R}}_+^q$, are possible ectropy functions for $\mathcal{G}$ with $\mathcal{E}_{\rm a}(0)=\mathcal{E}_{\rm r}(0)=0$. Finally, all ectropy functions $\mathcal{E}(V_{\rm s})$, $V_{\rm s}\in\overline{\mathbb{R}}_+^q$, for $\mathcal{G}$ satisfy

$$\mathcal{E}_{\rm a}(V_{\rm s}) \le \mathcal{E}(V_{\rm s})-\mathcal{E}(0) \le \mathcal{E}_{\rm r}(V_{\rm s}), \quad V_{\rm s}\in\overline{\mathbb{R}}_+^q, \quad (48)$$

Proof. The proof is similar to the proof of Theorem 3.1. □

The next proposition gives a closed-form expression for the ectropy of $\mathcal{G}$.

Proposition 3.6: Consider the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) and assume that Axiom $ii)$ holds. Then the function $\mathcal{E}:\overline{\mathbb{R}}_+^q\to\mathbb{R}$ given by

$$\mathcal{E}(V_{\rm s}) = \tfrac{1}{2}V_{\rm s}^{\rm T}V_{\rm s}, \quad V_{\rm s}\in\overline{\mathbb{R}}_+^q, \quad (49)$$

is an ectropy function of $\mathcal{G}$.

Proof. The proof is similar to the proof of Proposition 3.4. □

Remark 3.3: Note that the ectropy function given by (49) satisfies (45) as an equality for a reversible process and as a strict inequality for an irreversible process.

It follows from (49) that ectropy is a measure of the extent to which the system energy deviates from a homogeneous state. Thus, ectropy is the dual of entropy and is a measure of the tendency of the large-scale dynamical system $\mathcal{G}$ to do useful work and grow more organized.

Inequality (16) is precisely Clausius' inequality for reversible and irreversible thermodynamics as applied to large-scale dynamical systems; while inequality (45) is an anti Clausius inequality. Moreover, for the ectropy function defined by (49), it follows from Proposition 3.6 that a thermodynamically consistent large-scale dynamical system model is dissipative with respect to the supply rate $V_{\rm s}^{\rm T}S$ and with storage function corresponding to the system ectropy. For the entropy function given by (40) note that $\mathcal{S}(0)=0$ which is consistent with the *third law of thermodynamics* (Nernst's theorem) which states that the entropy of every system at absolute zero can always be taken to be equal to zero. For the isolated large-scale dynamical system $\mathcal{G}$, (16) yields the fundamental (universal) inequality

$$\mathcal{S}(V_{\rm s}(t_2)) \ge \mathcal{S}(V_{\rm s}(t_1)), \quad t_2\ge t_1. \quad (50)$$

Inequality (50) implies that, for any dynamical change in an isolated large-scale dynamical system $\mathcal{G}$, the entropy of the final state can never be less than the entropy of the initial state. It is important to stress that this result holds for an isolated dynamical system. It is however possible with power (heat flux) supplied from an external system to reduce the entropy of the dynamical system $\mathcal{G}$. The entropy of both systems taken together however cannot decrease. The above observations imply that when the isolated large-scale dynamical system $\mathcal{G}$ with thermodynamically consistent energy flow characteristics (i.e., Axioms $i)$ and $ii)$ hold) is at a state of maximum entropy consistent with its energy, it cannot be subject to any further dynamical change since any such change would result in a decrease of entropy. This of course implies that the state of *maximum entropy* is the stable state of an isolated system and this equilibrium state has to be semistable. Analogously, it follows from (45) that the isolated large-scale dynamical system $\mathcal{G}$ satisfies the fundamental inequality

$$\mathcal{E}(V_{\rm s}(t_2)) \le \mathcal{E}(V_{\rm s}(t_1)), \quad t_2\ge t_1, \quad (51)$$

which implies that the ectropy of the final state of $\mathcal{G}$ is always less than the ectropy of the initial state of $\mathcal{G}$. Hence, for the isolated large-scale dynamical system $\mathcal{G}$ the entropy increases if and only if the ectropy decreases. Thus, the state of *minimum ectropy* is the stable state of an isolated system and this equilibrium state has to be semistable. The next theorem concretizes the above observations.

Theorem 3.4: Consider the large-scale dynamical system $\mathcal{G}$ with power balance equation (6) with $S(t)\equiv 0$ and $d(V_{\rm s})\equiv 0$ and assume that Axioms $i)$ and $ii)$ hold. Then for every $\alpha\ge 0$, $\alpha\mathbf{e}$ is a semistable equilibrium state of (6). Furthermore, $V_{\rm s}(t)\to\frac{1}{q}\mathbf{e}\mathbf{e}^{\rm T}V_{\rm s}(t_0)$ as $t\to\infty$ and $\frac{1}{q}\mathbf{e}\mathbf{e}^{\rm T}V_{\rm s}(t_0)$ is a semistable equilibrium state. Finally, if for some $k\in\{1,\ldots,q\}$, $\sigma_{kk}(V_{\rm s})\ge 0$, $V_{\rm s}\in\overline{\mathbb{R}}_+^q$, and $\sigma_{kk}(V_{\rm s})=0$ if and only if $v_{{\rm s}k}=0$[2], then the zero solution $V_{\rm s}(t)\equiv 0$ to (6) is a globally asymptotically stable equilibrium state of (6).

Proof. It follows from Axiom $i)$ that $\alpha\mathbf{e}\in\overline{\mathbb{R}}_+^q$, $\alpha\ge 0$, is an equilibrium state for (6). To show Lyapunov stability of the equilibrium state $\alpha\mathbf{e}$ consider the system shifted ectropy function $\mathcal{E}_{\rm s}(V_{\rm s})=\frac{1}{2}(V_{\rm s}-\alpha\mathbf{e})^{\rm T}(V_{\rm s}-\alpha\mathbf{e})$ as a Lyapunov function candidate. Now, since $\phi_{ij}(V_{\rm s})=-\phi_{ji}(V_{\rm s})$, $V_{\rm s}\in$

[2]The assumption $\sigma_{kk}(V_{\rm s})\ge 0$, $V_{\rm s}\in\overline{\mathbb{R}}_+^q$, and $\sigma_{kk}(V_{\rm s})=0$ if and only if $v_{{\rm s}k}=0$ for some $k\in\{1,\ldots,q\}$ implies that if the kth subsystem possesses no energy, then this subsystem cannot dissipate energy to the environment. Conversely, if the kth subsystem does not dissipate energy to the environment, then this subsystem has no energy.

$\overline{\mathbb{R}}_+^q$, $i \neq j$, $i, j = 1, ..., q$, and $\mathbf{e}^{\mathrm{T}} w(V_{\mathrm{s}}) = 0$, $V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q$, it follows from Axiom ii) that

$$\begin{aligned}
\dot{\mathcal{E}}_{\mathrm{s}}(V_{\mathrm{s}}) &= (V_{\mathrm{s}} - \alpha\mathbf{e})^{\mathrm{T}} \dot{V}_{\mathrm{s}} \\
&= (V_{\mathrm{s}} - \alpha\mathbf{e})^{\mathrm{T}} w(V_{\mathrm{s}}) \\
&= V_{\mathrm{s}}^{\mathrm{T}} w(V_{\mathrm{s}}) \\
&= \sum_{i=1}^{q} v_{\mathrm{s}i} \left[\sum_{j=1,\, j\neq i}^{q} \phi_{ij}(V_{\mathrm{s}}) \right] \\
&= \sum_{i=1}^{q} \sum_{j=i+1}^{q} (v_{\mathrm{s}i} - v_{\mathrm{s}j}) \phi_{ij}(V_{\mathrm{s}}) \\
&= \sum_{i=1}^{q} \sum_{j\in\mathcal{K}_i} (v_{\mathrm{s}i} - v_{\mathrm{s}j}) \phi_{ij}(V_{\mathrm{s}}) \\
&\leq 0, \quad V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q,
\end{aligned} \tag{52}$$

where $\mathcal{K}_i \triangleq \mathcal{N}_i \setminus \cup_{l=1}^{i-1}\{l\}$ and $\mathcal{N}_i \triangleq \{j \in \{1, ..., q\} : \phi_{ij}(V_{\mathrm{s}}) = 0$ if and only if $v_{\mathrm{s}i} = v_{\mathrm{s}j}\}$, $i = 1, ..., q$, which establishes Lyapunov stability of the equilibrium state $\alpha\mathbf{e}$. To show that $\alpha\mathbf{e}$ is semistable, let $\mathcal{R} \triangleq \{V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q : \dot{\mathcal{E}}_{\mathrm{s}}(V_{\mathrm{s}}) = 0\} = \{V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q : (v_{\mathrm{s}i} - v_{\mathrm{s}j})\phi_{ij}(V_{\mathrm{s}}) = 0, i = 1, ..., q, j \in \mathcal{K}_i\}$. Now, by Axiom i) the directed graph associated with the connectivity matrix $\mathcal{C}$ for the large-scale dynamical system $\mathcal{G}$ is strongly connected which implies that $\mathcal{R} = \{V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q : v_{\mathrm{s}1} = \cdots = v_{\mathrm{s}q}\}$. Since the set $\mathcal{R}$ consists of the equilibrium states of (6), it follows that the largest invariant set $\mathcal{M}$ contained in $\mathcal{R}$ is given by $\mathcal{M} = \mathcal{R}$. Hence, it follows from the Krasovskii-LaSalle invariant set theorem [41] that for any initial condition $V_{\mathrm{s}}(t_0) \in \overline{\mathbb{R}}_+^q$, $V_{\mathrm{s}}(t) \to \mathcal{M}$ as $t \to \infty$ and hence $\alpha\mathbf{e}$ is a semistable equilibrium state of (6). Next, note that since $\mathbf{e}^{\mathrm{T}} V_{\mathrm{s}}(t) = \mathbf{e}^{\mathrm{T}} V_{\mathrm{s}}(t_0)$ and $V_{\mathrm{s}}(t) \to \mathcal{M}$ as $t \to \infty$, it follows that $V_{\mathrm{s}}(t) \to \frac{1}{q}\mathbf{e}\mathbf{e}^{\mathrm{T}} V_{\mathrm{s}}(t_0)$ as $t \to \infty$. Hence, with $\alpha = \frac{1}{q}\mathbf{e}^{\mathrm{T}} V_{\mathrm{s}}(t_0)$, $\alpha\mathbf{e} = \frac{1}{q}\mathbf{e}\mathbf{e}^{\mathrm{T}} V_{\mathrm{s}}(t_0)$ is a semistable equilibrium state of (6).

Finally, to show that in the case where for some $k \in \{1, ..., q\}$, $\sigma_{kk}(V_{\mathrm{s}}) \geq 0$, $V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q$, and $\sigma_{kk}(V_{\mathrm{s}}) = 0$ if and only if $v_{\mathrm{s}k} = 0$, the zero solution $V_{\mathrm{s}}(t) \equiv 0$ to (6) is globally asymptotically stable, consider the system ectropy $\mathcal{E}(V_{\mathrm{s}}) = \frac{1}{2} V_{\mathrm{s}}^{\mathrm{T}} V_{\mathrm{s}}$, $V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q$, as a candidate Lyapunov function. Note that $\mathcal{E}(0) = 0$, $\mathcal{E}(V_{\mathrm{s}}) > 0$, $V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q$, $V_{\mathrm{s}} \neq 0$, and $\mathcal{E}(V_{\mathrm{s}})$ is radially unbounded. Now, the Lyapunov derivative along the system energy trajectories of (6) is given by

$$\begin{aligned}
\dot{\mathcal{E}}(V_{\mathrm{s}}) &= V_{\mathrm{s}}^{\mathrm{T}} [w(V_{\mathrm{s}}) - d(V_{\mathrm{s}})] \\
&= V_{\mathrm{s}}^{\mathrm{T}} w(V_{\mathrm{s}}) - v_{\mathrm{s}k}\sigma_{kk}(V_{\mathrm{s}}) \\
&= \sum_{i=1}^{q} v_{\mathrm{s}i} \left[\sum_{j=1, j\neq i}^{q} \phi_{ij}(V_{\mathrm{s}}) \right] - v_{\mathrm{s}k}\sigma_{kk}(V_{\mathrm{s}}) \\
&= \sum_{i=1}^{q} \sum_{j=i+1}^{q} (v_{\mathrm{s}i} - v_{\mathrm{s}j}) \phi_{ij}(V_{\mathrm{s}}) - v_{\mathrm{s}k}\sigma_{kk}(V_{\mathrm{s}}) \\
&= \sum_{i=1}^{q} \sum_{j\in\mathcal{K}_i} (v_{\mathrm{s}i} - v_{\mathrm{s}j}) \phi_{ij}(V_{\mathrm{s}}) - v_{\mathrm{s}k}\sigma_{kk}(V_{\mathrm{s}}) \\
&\leq 0, \quad V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q,
\end{aligned} \tag{53}$$

which shows that the zero solution $V_{\mathrm{s}}(t) \equiv 0$ to (6) is Lyapunov stable. To show global asymptotic stability of the zero equilibrium state let $\mathcal{R} \triangleq \{V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q : \dot{\mathcal{E}}(V_{\mathrm{s}}) = 0\} = \{V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q : v_{\mathrm{s}k}\sigma_{kk}(V_{\mathrm{s}}) = 0, k \in \{1, ..., q\}\} \cap \{V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q : (v_{\mathrm{s}i} - v_{\mathrm{s}j})\phi_{ij}(V_{\mathrm{s}}) = 0, i = 1, ..., q, j \in \mathcal{K}_i\}$. Now, since Axiom i) holds and $\sigma_{kk}(V_{\mathrm{s}}) = 0$ if and only if $v_{\mathrm{s}k} = 0$ it follows that $\mathcal{R} = \{V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q : v_{\mathrm{s}k} = 0, k \in \{1, ..., q\}\} \cap \{V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q : v_{\mathrm{s}1} = v_{\mathrm{s}2} = \cdots = v_{\mathrm{s}q}\} = \{0\}$ and the largest invariant set $\mathcal{M}$ contained in $\mathcal{R}$ is given by $\mathcal{M} = \{0\}$. Hence, it follows from the Krasovskii-LaSalle invariant set theorem that for any initial condition $V_{\mathrm{s}}(t_0) \in \overline{\mathbb{R}}_+^q$, $V_{\mathrm{s}}(t) \to \mathcal{M} = \{0\}$ as $t \to \infty$ which proves global asymptotic stability of the zero equilibrium state of (6). □

In Theorem 3.4 we used the shifted ectropy function to show that for the isolated (i.e., $S(t) \equiv 0$ and $d(V_{\mathrm{s}}) \equiv 0$) large-scale dynamical system $\mathcal{G}$, $V_{\mathrm{s}}(t) \to \frac{1}{q}\mathbf{e}\mathbf{e}^{\mathrm{T}} V_{\mathrm{s}}(t_0)$ as $t \to \infty$ and $\frac{1}{q}\mathbf{e}\mathbf{e}^{\mathrm{T}} V_{\mathrm{s}}(t_0)$ is a semistable equilibrium state. This result can also be arrived at using the system entropy. To see this note that since $\mathbf{e}^{\mathrm{T}} w(V_{\mathrm{s}}) = 0$, $V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q$, it follows that $\mathbf{e}^{\mathrm{T}} \dot{V}_{\mathrm{s}}(t) = 0$, $t \geq t_0$. Hence, $\mathbf{e}^{\mathrm{T}} V_{\mathrm{s}}(t) = \mathbf{e}^{\mathrm{T}} V_{\mathrm{s}}(t_0)$, $t \geq t_0$. Furthermore, since $V_{\mathrm{s}}(t) \geq\geq 0$, $t \geq t_0$, it follows that $0 \leq\leq V_{\mathrm{s}}(t) \leq\leq \mathbf{e}\mathbf{e}^{\mathrm{T}} V_{\mathrm{s}}(t_0)$, $t \geq t_0$, which implies that all solutions to (6) are bounded. Next, since by (50) the entropy $\mathcal{S}(V_{\mathrm{s}}(t))$, $t \geq t_0$, of $\mathcal{G}$ is monotonically increasing and $V_{\mathrm{s}}(t)$, $t \geq t_0$, is bounded, the result follows using similar arguments as in Theorem 3.4.

Theorem 3.4 implies that the steady-state value of the energy in each subsystem $\mathcal{G}_i$ of the isolated large-scale dynamical system $\mathcal{G}$ is equal; that is, the steady-state energy of the isolated large-scale dynamical system $\mathcal{G}$ given by $V_{\mathrm{s}\,\infty} = \frac{1}{q}\mathbf{e}\mathbf{e}^{\mathrm{T}} V_{\mathrm{s}}(t_0) = \left[\frac{1}{q}\sum_{i=1}^{q} v_{\mathrm{s}i}(t_0)\right]\mathbf{e}$ is uniformly distributed over all subsystems of $\mathcal{G}$. This phenomenon is known as *equipartition of* energy[3] [23], [26], [29], [42], [43] and is an emergent behavior in thermodynamic systems. The next proposition shows that among all possible energy distributions in the large-scale dynamical system $\mathcal{G}$, energy equipartition corresponds to the minimum value of the system's ectropy and the maximum value of the system's entropy (see Figure 2).

Proposition 3.7: Consider the large-scale dynamical system $\mathcal{G}$ with power balance equation (6), let $\mathcal{E} : \overline{\mathbb{R}}_+^q \to \overline{\mathbb{R}}_+$ and $\mathcal{S} : \overline{\mathbb{R}}_+^q \to \mathbb{R}$ denote the ectropy and entropy of $\mathcal{G}$ given by (49) and (40), respectively, and define $\mathcal{D}_{\mathrm{c}} \triangleq \{V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q : \mathbf{e}^{\mathrm{T}} V_{\mathrm{s}} = \beta\}$, where $\beta \geq 0$. Then,

$$\arg\min_{V_{\mathrm{s}}\in\mathcal{D}_{\mathrm{c}}}(\mathcal{E}(V_{\mathrm{s}})) = \arg\max_{V_{\mathrm{s}}\in\mathcal{D}_{\mathrm{c}}}(\mathcal{S}(V_{\mathrm{s}})) = V_{\mathrm{s}}^* = \frac{\beta}{q}\mathbf{e}. \tag{54}$$

Furthermore, $\mathcal{E}_{\min} \triangleq \mathcal{E}(V_{\mathrm{s}}^*) = \frac{1}{2}\frac{\beta^2}{q}$ and $\mathcal{S}_{\max} \triangleq \mathcal{S}(V_{\mathrm{s}}^*) = q\log_e(c + \frac{\beta}{q}) - q\log_e c$.

Proof. The existence and uniqueness of V_{s}^* follows from the fact that $\mathcal{E}(V_{\mathrm{s}})$ and $-\mathcal{S}(V_{\mathrm{s}})$ are strictly convex continuous functions defined on the compact set $\mathcal{D}_{\mathrm{c}}$. To minimize $\mathcal{E}(V_{\mathrm{s}}) = \frac{1}{2}V_{\mathrm{s}}^{\mathrm{T}} V_{\mathrm{s}}$, $V_{\mathrm{s}} \in \overline{\mathbb{R}}_+^q$, subject to $V_{\mathrm{s}} \in \mathcal{D}_{\mathrm{c}}$ form the Lagrangian $\mathcal{L}(V_{\mathrm{s}}, \lambda) = \frac{1}{2}V_{\mathrm{s}}^{\mathrm{T}} V_{\mathrm{s}} + \lambda(\mathbf{e}^{\mathrm{T}} V_{\mathrm{s}} - \beta)$, where $\lambda \in \mathbb{R}$ is the Lagrange multiplier. If V_{s}^* solves this

[3]The phenomenon of equipartition of energy is closely related to the notion of a *monotemperaturic* system discussed in [25].

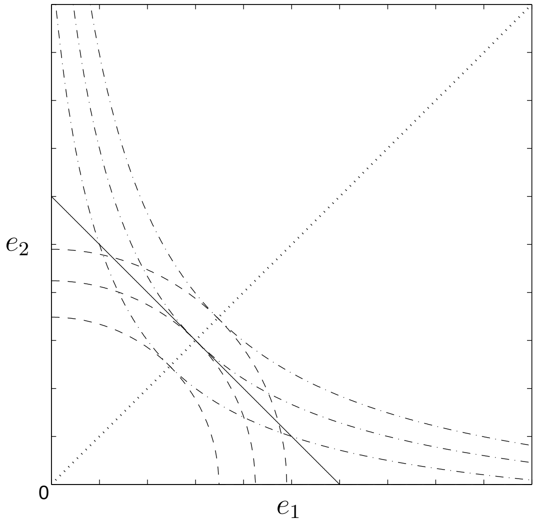

Fig. 2. Thermodynamic equilibria ($\cdots$), constant energy surfaces (———), constant ectropy surfaces ($- - -$), and constant entropy surfaces ($- \cdot - \cdot -$)

minimization problem, then

$$0 = \left.\frac{\partial \mathcal{L}}{\partial V_{\rm s}}\right|_{V_{\rm s}=V_{\rm s}^*} = V_{\rm s}^{*{\rm T}} + \lambda \mathbf{e}^{\rm T} = 0 \qquad (55)$$

and hence $V_{\rm s}^* = -\lambda \mathbf{e}$. Now, it follows from $\mathbf{e}^{\rm T} V_{\rm s} = \beta$ that $\lambda = -\frac{\beta}{q}$ which implies that $V_{\rm s}^* = \frac{\beta}{q}\mathbf{e} \in \overline{\mathbb{R}}_+^q$. The fact that $V_{\rm s}^*$ minimizes the ectropy on the compact set $\mathcal{D}_{\rm c}$ can be shown by computing the Hessian of the ectropy for the constrained parameter optimization problem and showing that the Hessian is positive definite at $V_{\rm s}^*$. $\mathcal{E}_{\min} = \frac{1}{2}\frac{\beta^2}{q}$ is now immediate.

Analogously, to maximize $\mathcal{S}(V_{\rm s}) = \mathbf{e}^{\rm T}\mathbf{log}_e(c\mathbf{e} + V_{\rm s}) - q \log_e c$ on the compact set $\mathcal{D}_{\rm c}$, form the Lagrangian $\mathcal{L}(V_{\rm s}, \lambda) \triangleq \sum_{i=1}^q \log_e(c + v_{{\rm s}i}) + \lambda(\mathbf{e}^{\rm T} V_{\rm s} - \beta)$, where $\lambda \in \mathbb{R}$ is a Largange multiplier. If $V_{\rm s}^*$ solves this maximization problem, then

$$\begin{aligned} 0 &= \left.\frac{\partial \mathcal{L}}{\partial V_{\rm s}}\right|_{V_{\rm s}=V_{\rm s}^*} \\ &= \left[\frac{1}{c + v_{{\rm s}1}^*} + \lambda, ..., \frac{1}{c + v_{{\rm s}q}^*} + \lambda\right] = 0. \qquad (56) \end{aligned}$$

Thus, $\lambda = -\frac{1}{c + v_{{\rm s}i}^*}$, $i = 1, ..., q$. If $\lambda = 0$, then the only value of $V_{\rm s}^*$ that satisfies (56) is $V_{\rm s}^* = \infty$, which does not satisfy the constraint equation $\mathbf{e}^{\rm T} V_{\rm s} = \beta$ for finite $\beta \geq 0$. Hence, $\lambda \neq 0$ and $v_{{\rm s}i}^* = -(\frac{1}{\lambda} + c)$, $i = 1, ..., q$, which implies $V_{\rm s}^* = -(\frac{1}{\lambda} + c)\mathbf{e}$. Now, it follows from $\mathbf{e}^{\rm T} V_{\rm s} = \beta$ that $-(\frac{1}{\lambda} + c) = \frac{\beta}{q}$ and hence $V_{\rm s}^* = \frac{\beta}{q}\mathbf{e} \in \overline{\mathbb{R}}_+^q$. The fact that $V_{\rm s}^*$ maximizes the entropy on the compact set $\mathcal{D}_{\rm c}$ can be shown by computing the Hessian and showing that it is negative definite at $V_{\rm s}^*$. $\mathcal{S}_{\max} = q \log_e(c + \frac{\beta}{q}) - q \log_e c$ is now immediate. $\square$

It follows from (50), (51), and Proposition 3.7 that conservation of energy necessarily implies nonconservation of ectropy and entropy. Hence, in an isolated large-scale dynamical system $\mathcal{G}$ all the energy, though always conserved, will eventually be degraded (diluted) to the point where it cannot produce any useful work. Hence, all motion would cease and the large-scale dynamical system would be fated to a state of eternal rest (semistability) wherein all subsystems will posses identical energies (energy equipartition). Ectropy would be a minimum and entropy would be a maximum giving rise to a state of absolute disorder. This is precisely what is known in theoretical physics as the *heat death of the universe*.

Next, we show that our thermodynamically consistent large-scale system $\mathcal{G}$ satisfies *Gibbs' principle* [44, p. 56]. Gibbs' version of the second law of thermodynamics can be stated as follows:

> **Gibbs' Principle.** *For an equilibrium of any isolated system it is necessary and sufficient that in all possible variations of the state of the system which do not alter its energy, the variation of its entropy shall either vanish or be negative.*

To establish Gibb's principle for our thermodynamically consistent energy flow model, suppose $E_{\rm e} = \alpha \mathbf{e}$, $\alpha \geq 0$, is an equilibrium point for the isolated system $\mathcal{G}$. Now, it follows from Proposition 3.7 that the entropy of $\mathcal{G}$ achieves its maximum at $E_{\rm e}$ subject to the constant energy level $\mathbf{e}^{\rm T} E = \alpha q$, $E \in \overline{\mathbb{R}}_+^q$. Hence, any variation of the state of the system which does not alter its energy leads to a zero or negative variation of the system entropy. Conversely, suppose at some point $E^* \in \overline{\mathbb{R}}_+^q$ the variation of the system entropy is either zero or negative for all possible variations in the state of the system which do not alter the system's total energy. Furthermore, *ad absurdum*, let the isolated system $\mathcal{G}$ undergo an irreversible transformation starting at E^*. Then it follows from Proposition 3.4 that the entropy of $\mathcal{G}$ given by (40) strictly increases which contradicts the above assumption. Hence, the system $\mathcal{G}$ cannot undergo an irreversible transformation starting at E^*. Alternatively, if the isolated system $\mathcal{G}$ undergoes a reversible transformation starting at E^*, then E^* has to be an equilibrium state of $\mathcal{G}$.

In the preceding discussion it was assumed that our large-scale dynamical system model is such that energy flows from more energetic subsystems to less energetic subsystems; that is, heat (energy) flows in the direction of lower temperatures. Although this universal phenomenon can be predicted with virtual certainty, it follows as a manifestation of entropy and ectropy nonconservation for the case of two subsystems. To see this, consider the isolated large-scale dynamical system $\mathcal{G}$ with power balance equation (6) (with $S(t) \equiv 0$ and $d(V_{\rm s}) \equiv 0$) and assume that the system entropy given by (40) is monotonically increasing and hence $\dot{\mathcal{S}}(V_{\rm s}(t)) \geq 0$, $t \geq t_0$. Now, since

$$\begin{aligned} \dot{\mathcal{S}}(V_{\rm s}(t)) &= \sum_{i=1}^q \frac{\dot{v}_{{\rm s}i}(t)}{c + v_{{\rm s}i}(t)} \\ &= \sum_{i=1}^q \sum_{j=1,\, j\neq i}^q \frac{\phi_{ij}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} \\ &= \sum_{i=1}^q \sum_{j=i+1}^q \left(\frac{\phi_{ij}(V_{\rm s}(t))}{c + v_{{\rm s}i}(t)} - \frac{\phi_{ij}(V_{\rm s}(t))}{c + v_{{\rm s}j}(t)}\right) \\ &= \sum_{i=1}^q \sum_{j\in\mathcal{K}_i} \frac{\phi_{ij}(V_{\rm s}(t))(v_{{\rm s}j}(t) - v_{{\rm s}i}(t))}{(c + v_{{\rm s}i}(t))(c + v_{{\rm s}j}(t))} \end{aligned}$$

$$\geq \quad 0, \quad t \geq t_0, \tag{57}$$

it follows that for $q = 2$, $(v_{s1} - v_{s2})\phi_{12}(V_s) \leq 0$, $V_s \in \overline{\mathbb{R}}_+^2$, which implies that energy (heat) flows naturally from a more energetic subsystem (hot object) to a less energetic subsystem (cooler object). The universality of this emergent behavior thus follows from the fact that entropy (respectively, ectropy) transfer, accompanying energy transfer, always increases (respectively, decreases). In the case where we have multiple subsystems, it is clear from (57) that entropy and ectropy nonconservation does not necessarily imply Axiom ii). However, if we invoke the additional condition (Axiom iii)) that if for any pair of connected subsystems $\mathcal{G}_k$ and $\mathcal{G}_l$, $k \neq l$, with $v_{sk} \geq v_{sl}$ (respectively, $v_{sk} \leq v_{sl}$) and for any other pair of connected subsystems $\mathcal{G}_m$ and $\mathcal{G}_n$, $m \neq n$, with $v_{sm} \geq v_{sn}$ (respectively, $v_{sm} \leq v_{sn}$) the inequality $\phi_{kl}(V_s)\phi_{mn}(V_s) \geq 0$, $V_s \in \overline{\mathbb{R}}_+^q$, holds, then nonconservation of entropy and ectropy in the isolated large-scale dynamical system $\mathcal{G}$ implies Axiom ii). The above inequality postulates that the direction of energy flow for any pair of *energy similar* subsystems is consistent; that is, if for a given pair of connected subsystems at a given energy level the energy flows in a certain direction, then for any other pair of connected subsystems with the same energy level, the energy flow direction is consistent with the original pair of subsystems. Note that this assumption does *not* specify the direction of energy flow between subsystems. To see that $\dot{\mathcal{S}}(V_s(t)) \geq 0$, $t \geq t_0$, along with Axiom iii) implies Axiom ii) note that since (57) holds for all $t \geq t_0$ and $V_s(t_0) \in \overline{\mathbb{R}}_+^q$ is arbitrary, (57) implies

$$\sum_{i=1}^{q} \sum_{j\in\mathcal{K}_i} \frac{\phi_{ij}(V_s)(v_{sj} - v_{si})}{(c + v_{si})(c + v_{sj})} \geq 0, \quad V_s \in \overline{\mathbb{R}}_+^q. \tag{58}$$

Now, it follows from (58) that for any fixed system energy level $V_s \in \overline{\mathbb{R}}_+^q$ there exists at least one pair of connected subsystems $\mathcal{G}_k$ and $\mathcal{G}_l$, $k \neq l$, such that $\phi_{kl}(V_s)(v_{sl} - v_{sk}) \geq 0$. Thus, if $v_{sk} \geq v_{sl}$ (respectively, $v_{sk} \leq v_{sl}$), then $\phi_{kl}(V_s) \leq 0$ (respectively, $\phi_{kl}(V_s) \geq 0$). Furthermore, it follows from Axiom iii) that for any other pair of connected subsystems $\mathcal{G}_m$ and $\mathcal{G}_n$, $m \neq n$, with $v_{sm} \geq v_{sn}$ (respectively, $v_{sm} \leq v_{sn}$) the inequality $\phi_{mn}(V_s) \leq 0$ (respectively, $\phi_{mn}(V_s) \geq 0$) holds which implies that

$$\phi_{mn}(V_s)(v_{sn} - v_{sm}) \geq 0, \quad m \neq n. \tag{59}$$

Thus, it follows from (59) that energy (heat) flows naturally from more energetic subsystems (hot objects) to less energetic subsystems (cooler objects). Of course, since in the isolated large-scale dynamical system $\mathcal{G}$ ectropy decreases if and only if entropy increases, the same result can be arrived at by considering the ectropy of $\mathcal{G}$. Since Axiom ii) holds, it follows from the conservation of energy and the fact that the large-scale dynamical system $\mathcal{G}$ is strongly connected that nonconservation of entropy and ectropy necessarily implies energy equipartition.

Finally, we close this section by showing that our definition of entropy given by (40) satisfies the eight criteria established in [45] for the acceptance of an analytic expression for representing a system entropy function. In particular, note that for a dynamical system $\mathcal{G}$: i) $\mathcal{S}(V_s)$ is well defined for every state $V_s \in \overline{\mathbb{R}}_+^q$ as long as $c > 0$. ii) If $\mathcal{G}$ is isolated, then $\mathcal{S}(V_s(t))$ is a nondecreasing function of time. iii) If $\mathcal{S}_i(v_{si}) = \log_e(c + v_{si}) - \log_e c$ is the entropy of the ith subsystem of the system $\mathcal{G}$, then $\mathcal{S}(V_s) = \sum_{i=1}^{q} \mathcal{S}_i(v_{si}) = \mathbf{e}^{\mathrm{T}}\mathbf{log}_e(c\mathbf{e} + V_s) - q\log_e c$ and hence the system entropy $\mathcal{S}(V_s)$ is an additive quantity over all subsystems. iv) For the system $\mathcal{G}$, $\mathcal{S}(V_s) \geq 0$ for all $V_s \in \overline{\mathbb{R}}_+^q$. v) It follows from Proposition 3.7 that for a given value $\beta \geq 0$ of the total energy of the system $\mathcal{G}$, one and only one state; namely, $V_s^* = \frac{\beta}{q}\mathbf{e}$, corresponds to the largest value of $\mathcal{S}(V_s)$. vi) It follows from (40) that for the system $\mathcal{G}$, graph of entropy versus energy is concave and smooth. vii) For a composite large-scale dynamical system $\mathcal{G}_C$ of two dynamical systems $\mathcal{G}_A$ and $\mathcal{G}_B$ the expression for the composite entropy $\mathcal{S}_C = \mathcal{S}_A + \mathcal{S}_B$, where $\mathcal{S}_A$ and $\mathcal{S}_B$ are entropies of $\mathcal{G}_A$ and $\mathcal{G}_B$, respectively, is such that the expression for the equilibrium state where the composite maximum entropy is achieved is identical to those obtained for $\mathcal{G}_A$ and $\mathcal{G}_B$ individually. Specifically, if q_A and q_B denote the number of subsystems in $\mathcal{G}_A$ and $\mathcal{G}_B$, respectively, and β_A and β_B denote the total energies of $\mathcal{G}_A$ and $\mathcal{G}_B$, respectively, then the maximum entropy of $\mathcal{G}_A$ and $\mathcal{G}_B$ individually is achieved at $V_{sA}^* = \frac{\beta_A}{q_A}\mathbf{e}$ and $V_{sB}^* = \frac{\beta_B}{q_B}\mathbf{e}$, respectively, while the maximum entropy of the composite system $\mathcal{G}_C$ is achieved at $V_{sC}^* = \frac{\beta_A + \beta_B}{q_A + q_B}\mathbf{e}$. $viii$) It follows from Theorem 3.4 that for a stable equilibrium state $V_s = \frac{\beta}{q}\mathbf{e}$, where $\beta \geq 0$ is the total energy of the system $\mathcal{G}$ and q is the number of subsystems of $\mathcal{G}$, the entropy is totally defined by β and q; that is, $\mathcal{S}(V_s) = q\log_e(c + \frac{\beta}{q}) - q\log_e c$. Dual criteria to the eight criteria outlined above can also be established for an analytic expression representing system ectropy.

IV. Temperature Equipartition and Boltzmann's Kinetic Theory of Gases

The thermodynamic axioms introduced in Section III postulate that subsystem energies are synonymous to subsystem temperatures. In this section, we generalize the results of Section III to the case where the subsystem energies are proportional to the subsystem temperatures with the proportionality constants representing the subsystem *specific heats*. In the case where the specific heats of all the subsystems are equal the results of this section specialize to those of Section III. To include temperature notions in our large-scale dynamical system model we replace Axioms i) and ii) of Section III by the following axioms. Let $\beta_i > 0$, $i = 1, \ldots, q$, denote the reciprocal of the specific heat of the ith subsystem $\mathcal{G}_i$ so that the (empirical) temperature in ith subsystem is given by $\hat{T}_i = \beta_i v_{si}$. Axiom i): For the connectivity matrix $\mathcal{C} \in \mathbb{R}^{q\times q}$ associated with the large-scale dynamical system $\mathcal{G}$ defined by (12) and (13), rank $\mathcal{C} = q - 1$ and for $\mathcal{C}_{(i,j)} = 1$, $i \neq j$, $\phi_{ij}(V_s) = 0$ if and only if $\beta_i v_{si} = \beta_j v_{sj}$. Axiom ii): For $i, j = 1, ..., q$, $(\beta_i v_{si} - \beta_j v_{sj})\phi_{ij}(V_s) \leq 0$, $V_s \in \overline{\mathbb{R}}_+^q$. Axiom i) implies that if the temperatures in the connected subsystems $\mathcal{G}_i$ and $\mathcal{G}_j$ are equal, then heat exchange between these subsystems is not possible. This is a statement of the zeroth law of thermodynamics which postulates that temperature equality is a necessary and sufficient condition for *thermal equilibrium*. Axiom ii) implies that heat (energy) must flow in the direction of lower temperatures. This is a statement of the second law of thermodynamics which states that a transformation whose only final result is to transfer heat from a body at a given temperature to a body at a higher temperature is impossible. Next, in light of our modified axioms we present a generalized definition for the entropy and ectropy of $\mathcal{G}$. The following proposition is needed for the statement of the main results of this section.

Proposition 4.1: Consider the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) and assume that Axiom ii) holds. Then for all $V_{s0} \in \overline{\mathbb{R}}_+^q$, $t_f \geq t_0$, and $S(t)$, $t \in [t_0, t_f]$, such that $V_s(t_f) = V_{s0}$,

$$\int_{t_0}^{t_f} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_s(t))}{c + \beta_i v_{si}(t)} dt = \oint \sum_{i=1}^{q} \frac{dQ_i(t)}{c + \beta_i v_{si}(t)} \leq 0, \quad (60)$$

and

$$\int_{t_0}^{t_f} \sum_{i=1}^{q} \beta_i v_{si}(t)[s_i(t) - \sigma_{ii}(V_s(t))] dt = \oint \sum_{i=1}^{q} \beta_i v_{si}(t) dQ_i(t) \geq 0, \quad (61)$$

where $V_s(t)$, $t \geq t_0$, is the solution to (6) with initial condition $V_s(t_0) = V_{s0}$.

Proof. The proof is identical to the proof of Propositions 3.2 and 3.5. □

Note that with the modified Axiom i) the isolated large-scale dynamical system $\mathcal{G}$ has equilibrium energy states given by $V_{s\,e} = \alpha p$, for $\alpha \geq 0$, where $p \triangleq [1/\beta_1, ..., 1/\beta_q]^T$. As in Section III, we define a reversible process as a process where the trajectory of the system $\mathcal{G}$ moves along the set of equilibria for the isolated system $\mathcal{G}$ and an irreversible process as a process that is not reversible. Thus, it follows from Axioms i) and ii) that inequalities (60) and (61) are satisfied as equalities for a reversible process and as strict inequalities for for an irreversible process.

Definition 4.1: For the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6), a function $\mathcal{S} : \overline{\mathbb{R}}_+^q \to \mathbb{R}$ satisfying

$$\mathcal{S}(V_s(t_2)) \geq \mathcal{S}(V_s(t_1)) + \int_{t_1}^{t_2} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_s(t))}{c + \beta_i v_{si}(t)} dt, \quad (62)$$

for any $t_2 \geq t_1 \geq t_0$ and $S(t)$, $t \in [t_1, t_2]$, is called the *entropy* of $\mathcal{G}$.

Definition 4.2: For the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6), a function $\mathcal{E} : \overline{\mathbb{R}}_+^q \to \mathbb{R}$ satisfying

$$\mathcal{E}(V_s(t_2)) \leq \mathcal{E}(V_s(t_1)) + \int_{t_1}^{t_2} \sum_{i=1}^{q} \beta_i v_{si}(t)[s_i(t) - \sigma_{ii}(V_s(t))] dt, \quad (63)$$

for any $t_2 \geq t_1 \geq t_0$ and $S(t)$, $t \in [t_1, t_2]$, is called the *ectropy* of $\mathcal{G}$.

For the next result define

$$\mathcal{S}_a(V_{s0}) \triangleq - \sup_{S(\cdot) \in \mathcal{U}_c,\, T \geq t_0} \int_{t_0}^{T} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_s(t))}{c + \beta_i v_{si}(t)} dt, \quad (64)$$

$$\mathcal{E}_a(V_{s0}) \triangleq - \inf_{S(\cdot) \in \mathcal{U}_c,\, T \geq t_0} \int_{t_0}^{T} \sum_{i=1}^{q} \beta_i v_{si}(t)[s_i(t) - \sigma_{ii}(V_s(t))] dt, \quad (65)$$

where $V_s(t_0) = V_{s0} \in \overline{\mathbb{R}}_+^q$ and $V_s(T) = 0$, and define the functions $\mathcal{S}_r : \overline{\mathbb{R}}_+^q \to \mathbb{R}$ and $\mathcal{E}_r : \overline{\mathbb{R}}_+^q \to \mathbb{R}$ by

$$\mathcal{S}_r(V_{s0}) \triangleq \sup_{S(\cdot) \in \mathcal{U}_r,\, T \geq -t_0} \int_{-T}^{t_0} \sum_{i=1}^{q} \frac{s_i(t) - \sigma_{ii}(V_s(t))}{c + \beta_i v_{si}(t)} dt, \quad (66)$$

$$\mathcal{E}_r(V_{s0}) \triangleq \inf_{S(\cdot) \in \mathcal{U}_r,\, T \geq -t_0} \int_{-T}^{t_0} \sum_{i=1}^{q} \beta_i v_{si}(t)[s_i(t) - \sigma_{ii}(V_s(t))] dt, \quad (67)$$

where $V_s(-T) = 0$ and $V_s(t_0) = V_{s0} \in \overline{\mathbb{R}}_+^q$.

Theorem 4.1: Consider the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) and assume that Axiom ii) holds. Then there exists an entropy and an ectropy function for $\mathcal{G}$. Moreover, $\mathcal{S}_a(V_s)$, $V_s \in \overline{\mathbb{R}}_+^q$, and $\mathcal{S}_r(V_s)$, $V_s \in \overline{\mathbb{R}}_+^q$, are possible entropy functions for $\mathcal{G}$ with $\mathcal{S}_a(0) = \mathcal{S}_r(0) = 0$, and $\mathcal{E}_a(V_s)$, $V_s \in \overline{\mathbb{R}}_+^q$, and $\mathcal{E}_r(V_s)$, $V_s \in \overline{\mathbb{R}}_+^q$, are possible ectropy functions for $\mathcal{G}$ with $\mathcal{E}_a(0) = \mathcal{E}_r(0) = 0$. Finally, all entropy functions $\mathcal{S}(V_s)$, $V_s \in \overline{\mathbb{R}}_+^q$, for $\mathcal{G}$ satisfy

$$\mathcal{S}_r(V_s) \leq \mathcal{S}(V_s) - \mathcal{S}(0) \leq \mathcal{S}_a(V_s), \quad V_s \in \overline{\mathbb{R}}_+^q, \quad (68)$$

and all ectropy functions $\mathcal{E}(V_s)$, $V_s \in \overline{\mathbb{R}}_+^q$, for $\mathcal{G}$ satisfy

$$\mathcal{E}_a(V_s) \leq \mathcal{E}(V_s) - \mathcal{E}(0) \leq \mathcal{E}_r(V_s), \quad V_s \in \overline{\mathbb{R}}_+^q. \quad (69)$$

Proof. The proof is identical to the proof of Theorems 3.1 and 3.3. □

For the statement of the next result define $p \triangleq [1/\beta_1, \cdots, 1/\beta_q]^T$ and $P \triangleq \mathrm{diag}[\beta_1, \cdots, \beta_q]$.

Proposition 4.2: Consider the large-scale dynamical system $\mathcal{G}$ with the power balance equation (6) and assume that Axiom ii) holds. Then the function $\mathcal{S} : \overline{\mathbb{R}}_+^q \to \mathbb{R}$ given by

$$\mathcal{S}(V_s) = p^T \mathbf{log}_e(c\mathbf{e} + PV_s) - \mathbf{e}^T p \log_e c, \quad V_s \in \overline{\mathbb{R}}_+^q, \quad (70)$$

where $\mathbf{log}_e(c\mathbf{e} + PV_s)$ denotes the vector natural logarithm given by $[\log_e(c+\beta_1 v_{s1}), ..., \log_e(c+\beta_q v_{sq})]^T$, is an entropy function of $\mathcal{G}$. Furthermore, the function $\mathcal{E} : \overline{\mathbb{R}}_+^q \to \mathbb{R}$ given by

$$\mathcal{E}(V_s) = \tfrac{1}{2} V_s^T P V_s, \quad V_s \in \overline{\mathbb{R}}_+^q, \quad (71)$$

is an ectropy function of $\mathcal{G}$.

Proof. The proof is identical to the proof of Propositions 3.4 and 3.6. □

Remark 4.1: As in Section III, it can be shown that the entropy and ectropy functions for $\mathcal{G}$ defined by (70) and (71) satisfy, respectively, (62) and (63) as equalities for a reversible process and as strict inequalities for an irreversible process.

Once again, inequality (62) is Clausius' inequality for reversible and irreversible thermodynamics; while inequality (63) is an anti Clausius inequality. Moreover, for the ectropy function given by (71) inequality (63) shows that a thermodynamically consistent large-scale dynamical system model is dissipative with respect to the supply rate $V_{\rm s}^{\rm T}PS$ and with storage function corresponding to the system ectropy $\mathcal{E}(V_{\rm s})$. In addition, if we let $\mathrm{d}Q_i(t) \triangleq [s_i(t) - \sigma_{ii}(V_{\rm s}(t))]\mathrm{d}t$, $i = 1, ..., q$, denote the infinitesimal amount of heat received or dissipated by the ith subsystem of $\mathcal{G}$ over the infinitesimal time interval $\mathrm{d}t$ at the *absolute* ith *subsystem temperature* $T_i \triangleq c + \beta_i v_{{\rm s}i}$, then it follows from (62) that the system entropy varies by an amount

$$\mathrm{d}\mathcal{S}(V_{\rm s}(t)) \geq \sum_{i=1}^{q} \frac{\mathrm{d}Q_i(t)}{c + \beta_i v_{{\rm s}i}(t)}, \quad t \geq t_0. \tag{72}$$

Finally, note that the nonconservation of entropy and ectropy equations (50) and (51), respectively, for isolated large-scale dynamical systems also hold for the more general definitions of entropy and ectropy given in Definitions 4.1 and 4.2. The following theorem is a generalization of Theorem 3.4.

Theorem 4.2: Consider the large-scale dynamical system $\mathcal{G}$ with power balance equation (6) with $S(t) \equiv 0$ and $d(V_{\rm s}) \equiv 0$ and assume that Axioms i) and ii) hold. Then for every $\alpha \geq 0$, αp is a semistable equilibrium state of (6). Furthermore, $V_{\rm s}(t) \to \frac{1}{\mathbf{e}^{\rm T}p} p\mathbf{e}^{\rm T}V_{\rm s}(t_0)$ as $t \to \infty$ and $\frac{1}{\mathbf{e}^{\rm T}p} p\mathbf{e}^{\rm T}V_{\rm s}(t_0)$ is a semistable equilibrium state. Finally, if for some $k \in \{1, ..., q\}$, $\sigma_{kk}(V_{\rm s}) \geq 0$ and $\sigma_{kk}(V_{\rm s}) = 0$ if and only if $v_{{\rm s}k} = 0$, then the zero solution $V_{\rm s}(t) \equiv 0$ to (6) is a globally asymptotically stable equilibrium state of (6).

Proof. It follows from Axiom i) that $\alpha p \in \overline{\mathbb{R}}_+^q$, $\alpha \geq 0$, is an equilibrium state for (6). To show Lyapunov stability of the equilibrium state αp consider the system shifted ectropy $\mathcal{E}_{\rm s}(V_{\rm s}) = \frac{1}{2}(V_{\rm s} - \alpha p)^{\rm T}P(V_{\rm s} - \alpha p)$ as a Lyapunov function candidate. Now, the proof follows as in the proof of Theorem 3.4 by invoking Axiom ii) and noting that $\phi_{ij}(V_{\rm s}) = -\phi_{ji}(V_{\rm s})$, $V_{\rm s} \in \overline{\mathbb{R}}_+^q$, $i \neq j, i, j = 1, ..., q$, $Pp = \mathbf{e}$, and $\mathbf{e}^{\rm T}w(V_{\rm s}) = 0$, $V_{\rm s} \in \overline{\mathbb{R}}_+^q$. Alternatively, in the case where for some $k \in \{1, ..., q\}$, $\sigma_{kk}(V_{\rm s}) \geq 0$ and $\sigma_{kk}(V_{\rm s}) = 0$ if and only if $v_{{\rm s}k} = 0$, global asymptotic stability of the zero solution $V_{\rm s}(t) \equiv 0$ to (6) follows from standard Lyapunov arguments using the system ectropy $\mathcal{E}(V_{\rm s}) = \frac{1}{2}V_{\rm s}^{\rm T}PV_{\rm s}$ as a candidate Lyapunov function. □

It follows from Theorem 4.2 that the steady-state value of the energy in each subsystem $\mathcal{G}_i$ of the isolated large-scale dynamical system $\mathcal{G}$ is given by $V_{{\rm s}\infty} = \frac{1}{\mathbf{e}^{\rm T}p} p\mathbf{e}^{\rm T}V_{\rm s}(t_0)$ which implies that $v_{{\rm s}i\infty} = \frac{1}{\beta_i \mathbf{e}^{\rm T}p}\mathbf{e}^{\rm T}V_{\rm s}(t_0)$ or, equivalently, $\hat{T}_{i\infty} = \beta_i v_{{\rm s}i\infty} = \frac{1}{\mathbf{e}^{\rm T}p}\mathbf{e}^{\rm T}V_{\rm s}(t_0)$. Hence, the steady state temperature of the isolated large-scale dynamical system $\mathcal{G}$ given by $\hat{T}_\infty = \frac{1}{\mathbf{e}^{\rm T}p}\mathbf{e}^{\rm T}V_{\rm s}(t_0)\mathbf{e}$ is uniformly distributed over all the subsystems of $\mathcal{G}$. This phenomenon is known as *temperature equipartition* in which all the system energy is eventually transformed into heat at a uniform temperature and hence all natural processes (system motions) would cease.

Proposition 4.3: Consider the large-scale dynamical system $\mathcal{G}$ with power balance equation (6), let $\mathcal{E} : \overline{\mathbb{R}}_+^q \to \overline{\mathbb{R}}_+$ and $\mathcal{S} : \overline{\mathbb{R}}_+^q \to \mathbb{R}$ denote the ectropy and entropy of $\mathcal{G}$ and be given by (71) and (70), respectively, and define $\mathcal{D}_{\rm c} \triangleq \{V_{\rm s} \in \overline{\mathbb{R}}_+^q : \mathbf{e}^{\rm T}V_{\rm s} = \beta\}$, where $\beta \geq 0$. Then,

$$\arg\min_{V_{\rm s}\in\mathcal{D}_{\rm c}}(\mathcal{E}(V_{\rm s})) = \arg\max_{V_{\rm s}\in\mathcal{D}_{\rm c}}(\mathcal{S}(V_{\rm s})) = V_{\rm s}^* = \frac{\beta}{\mathbf{e}^{\rm T}p}p. \tag{73}$$

Furthermore, $\mathcal{E}_{\min} \triangleq \mathcal{E}(V_{\rm s}^*) = \frac{1}{2}\frac{\beta^2}{\mathbf{e}^{\rm T}p}$ and $\mathcal{S}_{\max} \triangleq \mathcal{S}(V_{\rm s}^*) = \mathbf{e}^{\rm T}p\log_e(c + \frac{\beta}{\mathbf{e}^{\rm T}p}) - \mathbf{e}^{\rm T}p\log_e c$.

Proof. The proof is identical to the proof of Proposition 3.7 and hence is omitted. □

Proposition 4.3 shows that when all the energy of a large-scale dynamical system is transformed into heat at a uniform temperature, entropy is a maximum and ectropy is a minimum.

Next, we provide a kinetic theory interpretation of the (steady-state) expressions for entropy and ectropy presented in this section. Specifically, we assume that each subsystem $\mathcal{G}_i$ of the large-scale dynamical system $\mathcal{G}$ is a simple system consisting of an ideal gas with rigid walls. Furthermore, we assume that all subsystems $\mathcal{G}_i$ are divided by *diathermal walls* (i.e., walls that permit energy flow) and the overall dynamical system is a closed system; that is, the system is separated from the environment by a rigid adiabatic wall. In this case, $\beta_i = k/n_i$, $i = 1, \ldots, q$, where n_i, $i = 1, \ldots, q$, is the number of molecules in the ith subsystem and $k > 0$ is the *Boltzmann constant* (i.e., gas constant per molecule). Without loss of generality and for simplicity of exposition let $k = 1$. In addition, we assume that the molecules in the ideal gas are hard elastic spheres; that is, there are no forces between the molecules except during collisions and the molecules are not deformed by collisions. Thus, there is no internal potential energy and the system internal energy of the ideal gas is entirely kinetic. Hence, in this case, the temperature of each subsystem $\mathcal{G}_i$ is the average translational kinetic energy per molecule which is consistent with the kinetic theory of ideal gases.

Definition 4.3: For a given isolated large-scale dynamical system $\mathcal{G}$ in *thermal equilibrium* define the *equilibrium entropy* of $\mathcal{G}$ by $\mathcal{S}_{\rm e} = n\log_e(c + \frac{\mathbf{e}^{\rm T}V_{{\rm s}\infty}}{n}) - n\log_e c$ and the *equilibrium ectropy* of $\mathcal{G}$ by $\mathcal{E}_{\rm e} = \frac{1}{2}\frac{(\mathbf{e}^{\rm T}V_{{\rm s}\infty})^2}{n}$, where $\mathbf{e}^{\rm T}V_{{\rm s}\infty}$ denotes the total steady-state energy of the large-scale dynamical system $\mathcal{G}$ and n denotes the number of molecules in $\mathcal{G}$.

Note that the equilibrium entropy and ectropy in Definition 4.3 is entirely consistent with the equilibrium (maximum) entropy and equilibrium (minimum) ectropy given by Proposition 4.3. Next, assume that each subsystem $\mathcal{G}_i$ is initially in thermal equilibrium. Furthermore, for each subsystem, let $v_{{\rm s}i}$ and n_i, $i = 1, ..., q$, denote the total internal energy and the number of molecules, respectively, in the ith subsystem. Hence, the entropy and ectropy of the ith subsystem are given by $\mathcal{S}_i = n_i\log_e(c + v_{{\rm s}i}/n_i) - n_i\log_e c$ and $\mathcal{E}_i = \frac{1}{2}\frac{v_{{\rm s}i}^2}{n_i}$, respectively. Next, note that the entropy and the ectropy of the overall system (after reaching a thermal equilibrium) are given by $\mathcal{S}_{\rm e} = n\log_e(c + \frac{\mathbf{e}^{\rm T}V_{{\rm s}\infty}}{n}) - n\log_e c$ and $\mathcal{E}_{\rm e} = \frac{1}{2}\frac{(\mathbf{e}^{\rm T}V_{{\rm s}\infty})^2}{n}$. Now, it follows from the convexity of $-\log_e(\cdot)$ and conservation of energy that the entropy of $\mathcal{G}$ at thermal equilibrium is given by

$$\mathcal{S}_{\rm e} \;=\; n\log_e\left(c + \frac{\mathbf{e}^{\rm T}V_{{\rm s}\infty}}{n}\right) - n\log_e c$$

$$= n\log_e\left[\sum_{i=1}^{q}\frac{n_i}{n}\left(c+\frac{v_{si}}{n_i}\right)\right]-\sum_{i=1}^{q}n_i\log_e c$$
$$\geq n\sum_{i=1}^{q}\frac{n_i}{n}\log_e\left(c+\frac{v_{si}}{n_i}\right)-\sum_{i=1}^{q}n_i\log_e c$$
$$= \sum_{i=1}^{q}\mathcal{S}_i. \quad (74)$$

Furthermore, the ectropy of $\mathcal{G}$ at thermal equilibrium is given by

$$\mathcal{E}_\mathrm{e} = \frac{1}{2}\frac{(\mathbf{e}^\mathrm{T}V_{\mathrm{s}\infty})^2}{n}$$
$$= \sum_{i=1}^{q}\frac{1}{2}\frac{v_{si}^2}{n_i}-\frac{1}{2n}\sum_{i=1}^{q}\sum_{j=i+1}^{q}\frac{(n_j v_{si}-n_i v_{sj})^2}{n_i n_j}$$
$$\leq \sum_{i=1}^{q}\frac{1}{2}\frac{v_{si}^2}{n_i}$$
$$= \sum_{i=1}^{q}\mathcal{E}_i. \quad (75)$$

It follows from (74) (respectively, (75)) that the equilibrium entropy (respectively, ectropy) of the system (gas) $\mathcal{G}$ is always greater (respectively, less) than the sum of entropies (respectively, ectropies) of the individual subsystems $\mathcal{G}_i$. Hence, the entropy (respectively, ectropy) of the gas increases (respectively, decreases) as a more evenly distributed (disordered) state is reached. Finally, note that it follows from (74) and (75) that $\mathcal{S}_\mathrm{e} = \sum_{i=1}^{q}\mathcal{S}_i$ and $\mathcal{E}_\mathrm{e}=\sum_{i=1}^{q}\mathcal{E}_i$ if and only if $\frac{v_{si}}{n_i}=\frac{v_{sj}}{n_j}$, $i\neq j$, $i,j=1,...,q$; that is, the initial temperatures of all subsystems are equal.

V. Thermodynamic Systems with Linear Energy Exchange

In this section we specialize the results of Section III to the case of linear energy exchange between subsystems; that is, $\sigma_{ij}(V_\mathrm{s})=\sigma_{ij}v_{sj}$, $\sigma_{ij}\geq 0$, $i,j=1,...,q$. In this case, the vector form of the energy balance equation (2), with $t_0=0$, is given by

$$V_\mathrm{s}(T)=V_\mathrm{s}(0)+\int_0^T WV_\mathrm{s}(t)\mathrm{d}t+\int_0^T S(t)\mathrm{d}t, \quad T\geq 0, \quad (76)$$

or, in power balance form,

$$\dot V_\mathrm{s}(t)=WV_\mathrm{s}(t)+S(t),\quad V_\mathrm{s}(0)=V_{\mathrm{s}0},\quad t\geq 0, \quad (77)$$

where $W\in\mathbb{R}^{q\times q}$ is such that

$$W_{(i,j)}=\begin{cases}-\sum_{k=1}^{q}\sigma_{kj}, & i=j,\\ \sigma_{ij}, & i\neq j.\end{cases} \quad (78)$$

Note that (78) implies $\sum_{i=1}^{q}W_{(i,j)}=-\sigma_{jj}\leq 0$, $j=1,...,q$, and hence W is a semistable compartmental matrix. If $\sigma_{ii}>0$, $i=1,...,q$, then W is an asymptotically stable compartmental matrix. An important special case of (77) is the case where W is symmetric or, equivalently, $\sigma_{ij}=\sigma_{ji}$, $i\neq j$, $i,j=1,...,q$. In this case, it follows from (77) that for each subsystem the power balance equation satisfies

$$\dot v_{si}(t)+\sigma_{ii}v_{si}(t)+\sum_{j=1,\,j\neq i}^{q}\sigma_{ij}[v_{si}(t)-v_{sj}(t)]=s_i(t) \quad (79)$$

for all $t\geq 0$. Note that $\phi_i(V_\mathrm{s})\triangleq\sum_{j=1,\,j\neq i}^{q}\sigma_{ij}[v_{si}-v_{sj}]$, $V_\mathrm{s}\in\overline{\mathbb{R}}_+^q$, $i=1,...,q$, represents the energy flow from the ith subsystem to all other subsystems and is given by the sum of the individual energy flows from the ith subsystem to the jth subsystem. Furthermore, these energy flows are proportional to the energy differences of the subsystems; that is, $v_{si}-v_{sj}$. Hence, (79) is a power balance equation that governs the energy exchange among coupled subsystems and is completely analogous to the equations of thermal transfer with subsystem energies playing the role of temperatures. Furthermore, note that since $\sigma_{ij}\geq 0$, $i\neq j$, $i,j=1,...,q$, energy flows from more energetic subsystems to less energetic subsystems which is consistent with the second law of thermodynamics which requires that heat (energy) *must* flow in the direction of lower temperatures.

The next proposition is needed for developing expressions for steady-state energy distributions of the large-scale dynamical system $\mathcal{G}$ with linear power balance equation (77).

Proposition 5.1 ([24]): Consider the large-scale dynamical system $\mathcal{G}$ with power balance equation given by (77). Suppose $V_{\mathrm{s}0}\geq\geq 0$ and $S(t)\geq\geq 0$, $t\geq 0$. Then the solution $V_\mathrm{s}(t)$, $t\geq 0$, to (77) is nonnegative for all $t\geq 0$ if and only if W is essentially nonnegative.

Next, we develop expressions for the steady-state energy distribution for the large-scale dynamical system $\mathcal{G}$ for the cases where supplied system power $S(t)$ is a periodic function with period $\tau>0$; that is, $S(t+\tau)=S(t)$, $t\geq 0$, and $S(t)$ is constant; that is, $S(t)\equiv S$. Define $e(t)\triangleq V_\mathrm{s}(t)-V_\mathrm{s}(t+\tau)$, $t\geq 0$, and note that

$$\dot e(t)=We(t),\quad e(0)=V_\mathrm{s}(0)-V_\mathrm{s}(\tau),\quad t\geq 0. \quad (80)$$

Hence, since

$$e(t)=e^{Wt}[V_\mathrm{s}(0)-V_\mathrm{s}(\tau)],\quad t\geq 0, \quad (81)$$

and W is semistable, it follows from $iv)$ of Lemma 2 of [23] that

$$\lim_{t\to\infty}e(t) = \lim_{t\to\infty}[V_\mathrm{s}(t)-V_\mathrm{s}(t+\tau)] = (I_q-WW^\#)[V_\mathrm{s}(0)-V_\mathrm{s}(\tau)], \quad (82)$$

which represents a constant offset to the steady-state error energy distribution in the large-scale dynamical system $\mathcal{G}$. For the case where $S(t)\equiv S$, $\tau\to\infty$ and hence the following result is immediate. This result first appeared in [23].

Proposition 5.2: Consider the large-scale dynamical system $\mathcal{G}$ with power balance equation given by (77). Suppose that $V_{\mathrm{s}0}\geq\geq 0$ and $S(t)\equiv S\geq\geq 0$. Then $V_{\mathrm{s}\infty}\triangleq\lim_{t\to\infty}V_\mathrm{s}(t)$ exists if and only if $S\in\mathcal{R}(W)$. In this case,

$$V_{\mathrm{s}\infty}=(I_q-WW^\#)V_{\mathrm{s}0}-W^\# S \quad (83)$$

and $V_{\mathrm{s}\infty}\geq\geq 0$. If, in addition, W is nonsingular, then $V_{\mathrm{s}\infty}$ exists for all $S\geq\geq 0$ and is given by

$$V_{\mathrm{s}\infty}=-W^{-1}S. \quad (84)$$

Proof. Note that it follows from Lagrange's formula that the solution $V_{\rm s}(t)$, $t \geq 0$, to (77) is given by

$$V_{\rm s}(t) = e^{Wt}V_{\rm s0} + \int_0^t e^{W(t-s)}S(s){\rm d}s, \quad t \geq 0. \qquad (85)$$

Now, the result is a direct consequence of Proposition 5.1 and $iv)$, $vii)$, $viii)$, and $ix)$ of Lemma 2 of [23]. □

Next, we specialize the result of Proposition 5.2 to the case where there is no energy dissipation from each subsystem $\mathcal{G}_i$ of $\mathcal{G}$; that is, $\sigma_{ii} = 0$, $i = 1, ..., q$. Note that in this case $\mathbf{e}^{\rm T}W = 0$ and hence rank $W \leq q-1$. Furthermore, if $S = 0$ it follows from (77) that $\mathbf{e}^{\rm T}\dot{V}_{\rm s}(t) = \mathbf{e}^{\rm T}WV_{\rm s}(t) = 0$, $t \geq 0$, and hence the total energy of the isolated large-scale dynamical system $\mathcal{G}$ is conserved.

Proposition 5.3: Consider the large-scale dynamical system $\mathcal{G}$ with power balance equation given by (77). Assume rank $W = q-1$, $\sigma_{ii} = 0$, $i = 1, ..., q$, and $W\mathbf{e} = 0$. If $V_{\rm s0} \geq\geq 0$ and $S = 0$, then the steady-state energy distribution $V_{\rm s\,\infty}$ of the isolated large-scale dynamical system $\mathcal{G}$ is given by

$$V_{\rm s\,\infty} = \left[\frac{1}{q}\sum_{i=1}^{q} v_{{\rm s}i0}\right]\mathbf{e}. \qquad (86)$$

Proof. The proof is similar to the proof of Theorem 3.4 with $w(V_{\rm s}) = WV_{\rm s}$. □

Finally, we examine the steady-state energy distribution for the large-scale dynamical system $\mathcal{G}$ in case of strong coupling between subsystems; that is, $\sigma_{ij} \to \infty$, $i \neq j$. For this analysis we assume that W given by (78) is symmetric; that is, $\sigma_{ij} = \sigma_{ji}$, $i \neq j$, $i, j = 1, ..., q$, and $\sigma_{ii} > 0$, $i = 1, ..., q$. Thus, $-W$ is a nonsingular M-matrix for all values of σ_{ij}, $i \neq j$, $i, j = 1, ..., q$. Moreover, in this case it can be shown that if $\frac{\sigma_{ij}}{\sigma_{kl}} \to 1$ as $\sigma_{ij} \to \infty$, $i \neq j$, and $\sigma_{kl} \to \infty$, $k \neq l$, then

$$\lim_{\sigma_{ij}\to\infty,\, i\neq j} W^{-1} = -\frac{1}{\sum_{i=1}^{q}\sigma_{ii}}\mathbf{e}\mathbf{e}^{\rm T}. \qquad (87)$$

Hence, in the limit of strong coupling the steady-state energy distribution $V_{\rm s\,\infty}$ given by (84) becomes

$$V_{\rm s\,\infty} = \lim_{\sigma_{ij}\to\infty,\, i\neq j}(-W^{-1}S) = \left[\frac{\mathbf{e}^{\rm T}S}{\sum_{i=1}^{q}\sigma_{ii}}\right]\mathbf{e}, \qquad (88)$$

which implies energy equipartition. This result first appeared in [23].

VI. Continuum Thermodynamics

In this section we extend the results of Section III to the case of continuous thermodynamic systems wherein the subsystems are uniformly distributed over an n dimensional space. Since these systems involve distributed subsystems they are described by partial differential equations and hence are infinite dimensional systems. Specifically, we consider continuous dynamical systems $\mathcal{G}$ defined over a compact connected set $\mathcal{V} \subset \mathbb{R}^n$ with a smooth (at least C^1) boundary $\partial\mathcal{V}$ and volume $\mathcal{V}_{\rm vol}$. Furthermore, let $\mathcal{X}$ denote a space of two-times continuously differentiable scalar functions defined on $\mathcal{V}$, let $v(x,t)$, where $v : \mathcal{V}\times\overline{\mathbb{R}}_+ \to \overline{\mathbb{R}}_+$, denote the energy density of the dynamical system $\mathcal{G}$ at the point $x \triangleq [x_1, ..., x_n]^{\rm T} \in \mathcal{V}$ and time instant $t \geq t_0$, let $\phi : \mathcal{V} \times \overline{\mathbb{R}}_+ \times \mathbb{R}^n \to \mathbb{R}^n$ denote the system energy flow within the continuum $\mathcal{V}$; that is, $\phi(x, v(x,t), \nabla v(x,t)) = [\phi_1(x, v(x,t), \nabla v(x,t)), ..., \phi_n(x, v(x,t), \nabla v(x,t))]^{\rm T}$, where $\phi_i(\cdot,\cdot,\cdot)$ denotes the energy flow through a unit area per unit time in the x_i direction for all $i = 1, ..., n$ and $\nabla v(x,t) \triangleq [D_1 v(x,t), ..., D_n v(x,t)]$, $x \in \mathcal{V}$, $t \geq t_0$, denotes the gradient of $v(\cdot,t)$ with respect to the spatial variable x, and let $s : \mathcal{V} \times \overline{\mathbb{R}}_+ \to \overline{\mathbb{R}}_+$ denote the energy (heat) flow into a unit volume per unit time from sources uniformly distributed over $\mathcal{V}$. Hence, a power balance equation over a unit volume within the continuum $\mathcal{V}$ involving the rate of energy density change, the external supplied power (heat flux), and the energy (heat) flow within the continuum yields

$$\frac{\partial v(x,t)}{\partial t} = -\nabla\cdot\phi(x, v(x,t), \nabla v(x,t)) + s(x,t), \quad t \geq t_0, \qquad (89)$$

$$v(x,t_0) = v_0(x), \quad x \in \mathcal{V},$$
$$\phi(x, v(x,t), \nabla v(x,t))\cdot\hat{n}(x) \geq 0, \quad x \in \partial\mathcal{V}, \quad t \geq t_0, \qquad (90)$$

where ∇ denotes the nabla operator, $\hat{n}(x)$ denotes the outward normal vector to the boundary $\partial\mathcal{V}$ (at x) of the set $\mathcal{V}$, "·" denotes the dot product in $\mathbb{R}^n$, and $v_0(\cdot) \in \mathcal{X}$ is a given initial energy density distribution. The power balance (conservation) equation (89) describes the time evolution of the energy density $v(x,t)$ over the region $\mathcal{V}$ while the boundary condition in (90) involving the dot product implies that the energy of the system $\mathcal{G}$ can either be stored or dissipated but not supplied through the boundary of $\mathcal{V}$. Furthermore, we denote the energy density distribution over the set $\mathcal{V}$ at time $t \geq t_0$ by $v_t \in \mathcal{X}$ so that for each $t \geq t_0$ the set of mappings generated by $v_t(x) \equiv v(x,t)$ for every $x \in \mathcal{V}$ gives the flow of $\mathcal{G}$. We assume that the function $\phi(\cdot,\cdot,\cdot)$ is continuously differentiable so that (89), (90) admits a unique solution $v(x,t)$, $x \in \mathcal{V}$, $t \geq t_0$, and $v(\cdot,t) \in \mathcal{X}$, $t \geq t_0$, is continuously dependent on initial energy density distribution $v_0(x)$, $x \in \mathcal{V}$. It is well known that if (89) is strictly parabolic, and $v_0(\cdot)$ is a C^2 function with compact support and its derivative is sufficiently small on $[t_0, \infty)$, then the classical solution to (89), (90) breaks down at a finite time. As a consequence of this, one may only hope to find generalized (or weak) solutions to (89), (90) over the semi-infinite interval $[t_0, \infty)$, that is, L_∞ functions $v(\cdot,\cdot)$ that satisfy (89) in the sense of distributions.

As in Section III, to ensure a thermodynamically consistent energy flow infinite dimensional model we require the following axioms analogous to Axioms $i)$ and $ii)$. Axiom $i)'$: For every $x \in \mathcal{V}$ and unit vector $\mathbf{u} \in \mathbb{R}^n$, $\phi(x, v_t(x), \nabla v_t(x))\cdot\mathbf{u} = 0$ if and only if $\nabla v_t(x)\mathbf{u} = 0$. Axiom $ii)'$: For every $x \in \mathcal{V}$ and unit vector $\mathbf{u} \in \mathbb{R}^n$, $\phi(x, v_t(x), \nabla v_t(x))\cdot\mathbf{u} > 0$ if and only if $\nabla v_t(x)\mathbf{u} < 0$, and $\phi(x, v_t(x), \nabla v_t(x))\cdot\mathbf{u} < 0$ if and only if $\nabla v_t(x)\mathbf{u} > 0$. Note that Axiom $i)'$ implies that $\phi_i(x, v_t(x), \nabla v_t(x)) = 0$ if and only if $D_i v_t(x) = 0$, $x \in \mathcal{V}$, $i = 1, ..., n$, while Axiom $ii)'$ implies that $\phi_i(x, v_t(x), \nabla v_t(x))D_i v_t(x) \leq 0$, $x \in \mathcal{V}$, $i = 1, ..., n$, which further implies that $\nabla v_t(x)\phi(x, v_t(x), \nabla v_t(x)) \leq 0$, $x \in \mathcal{V}$; that is, energy (heat) flows from regions of higher to lower energy densities. If $s(x,t) \equiv 0$, then Axioms $i)'$ and $ii)'$ along with the fact that $\phi(x, v(x,t), \nabla v(x,t))\cdot\hat{n}(x) \geq 0$, $x \in \partial\mathcal{V}$, $t \geq t_0$, imply that at a given instant of time the energy of the dynamical system $\mathcal{G}$ can only be transported, stored, or dissipated but not created. Next, we establish the classical Clausius inequality for our thermodynamically consistent infinite dimensional energy flow model given by (89), (90). For the remainder of this section $\mathrm{d}\mathcal{V}$ represents an infinitesimal volume element of $\mathcal{V}$, $\mathcal{S}_{\mathcal{V}}$ denotes the surface enclosing $\mathcal{V}$ and $\mathrm{d}\mathcal{S}_{\mathcal{V}}$ denotes an infinitesimal boundary element.

Proposition 6.1: Consider the dynamical system $\mathcal{G}$ with the power balance equation (89), (90) and assume that Axiom $ii)'$ holds. Then, for every initial energy density distribution $v_0(\cdot) \in \mathcal{X}$, $t_{\mathrm{f}} \geq t_0$, and $s(t)$, $t \in [t_0, t_{\mathrm{f}}]$, such that $v_{t_{\mathrm{f}}}(x) \equiv v_0(x)$,

$$\int_{t_0}^{t_{\mathrm{f}}} \int_{\mathcal{V}} \frac{s(x,t)}{c+v(x,t)} \mathrm{d}\mathcal{V}\, \mathrm{d}t - \int_{t_0}^{t_{\mathrm{f}}} \int_{\partial\mathcal{V}} \frac{\phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x)}{c+v(x,t)} \mathrm{d}\mathcal{S}_{\mathcal{V}}\, \mathrm{d}t \leq 0, \quad (91)$$

where $c > 0$ and $v(x,t)$, $x \in \mathcal{V}, t \geq t_0$, is the solution to (89), (90).

Proof. It follows from the Green-Gauss theorem and Axiom $ii)'$ that

$$\begin{aligned}
&\int_{t_0}^{t_{\mathrm{f}}} \int_{\mathcal{V}} \frac{s(x,t)}{c+v(x,t)} \mathrm{d}\mathcal{V}\mathrm{d}t \\
&\qquad - \int_{t_0}^{t_{\mathrm{f}}} \int_{\partial\mathcal{V}} \frac{\phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x)}{c+v(x,t)} \mathrm{d}\mathcal{S}_{\mathcal{V}}\mathrm{d}t \\
&= \int_{t_0}^{t_{\mathrm{f}}} \int_{\mathcal{V}} \frac{\frac{\partial v(x,t)}{\partial t} + \nabla \cdot \phi(x, v(x,t), \nabla v(x,t))}{c+v(x,t)} \mathrm{d}\mathcal{V}\mathrm{d}t \\
&\qquad - \int_{t_0}^{t_{\mathrm{f}}} \int_{\partial\mathcal{V}} \frac{\phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x)}{c+v(x,t)} \mathrm{d}\mathcal{S}_{\mathcal{V}}\mathrm{d}t \\
&= \int_{\mathcal{V}} \log_e \left(\frac{c+v(x,t_{\mathrm{f}})}{c+v_0(x)} \right) \mathrm{d}\mathcal{V} \\
&\qquad + \int_{t_0}^{t_{\mathrm{f}}} \int_{\partial\mathcal{V}} \frac{\phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x)}{c+v(x,t)} \mathrm{d}\mathcal{S}_{\mathcal{V}}\mathrm{d}t \\
&\qquad + \int_{t_0}^{t_{\mathrm{f}}} \int_{\mathcal{V}} \frac{\nabla v(x,t) \phi(x, v(x,t), \nabla v(x,t))}{(c+v(x,t))^2} \mathrm{d}\mathcal{V}\mathrm{d}t \\
&\qquad - \int_{t_0}^{t_{\mathrm{f}}} \int_{\partial\mathcal{V}} \frac{\phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x)}{c+v(x,t)} \mathrm{d}\mathcal{S}_{\mathcal{V}}\mathrm{d}t \\
&= \int_{t_0}^{t_{\mathrm{f}}} \int_{\mathcal{V}} \frac{\nabla v(x,t) \phi(x, v(x,t), \nabla v(x,t))}{(c+v(x,t))^2} \mathrm{d}\mathcal{V}\mathrm{d}t \\
&\leq 0, \qquad (92)
\end{aligned}$$

which proves the result. □

Next, we give the entropy definition for continuous dynamical systems.

Definition 6.1: For the dynamical system $\mathcal{G}$ with the power balance equation (89), (90), the function $\mathcal{S} : \mathcal{X} \to \mathbb{R}$ satisfying

$$\mathcal{S}(v_{t_2}) \geq \mathcal{S}(v_{t_1}) + \int_{t_1}^{t_2} q(t) \mathrm{d}t, \quad (93)$$

for all $s(t)$, $t \geq t_0$, and $t_2 \geq t_1 \geq t_0$, where

$$q(t) \triangleq \int_{\mathcal{V}} \frac{s(x,t)}{c+v(x,t)} \mathrm{d}\mathcal{V} - \int_{\partial\mathcal{V}} \frac{\phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x)}{c+v(x,t)} \mathrm{d}\mathcal{S}_{\mathcal{V}} \quad (94)$$

and $c > 0$, is called the *entropy* of $\mathcal{G}$.

Theorem 6.1: Consider the dynamical system $\mathcal{G}$ with the power balance equation (89), (90) and assume that Axiom $ii)'$ holds. Then the function $\mathcal{S} : \mathcal{X} \to \mathbb{R}$ given by

$$\mathcal{S}(v_t) = \int_{\mathcal{V}} \log_e(c + v_t(x)) \mathrm{d}\mathcal{V} - \mathcal{V}_{\mathrm{vol}} \log_e c, \quad (95)$$

is an entropy function for $\mathcal{G}$.

Proof. It follows from the Green-Gauss theorem, Axiom $ii)'$, and (95) that

$$\begin{aligned}
\dot{\mathcal{S}}(v_t) &= \int_{\mathcal{V}} \frac{1}{c+v(x,t)} \frac{\partial v(x,t)}{\partial t} \mathrm{d}\mathcal{V} \\
&= \int_{\mathcal{V}} \frac{(-\nabla \cdot \phi(x, v(x,t), \nabla v(x,t)) + s(x,t))}{c+v(x,t)} \mathrm{d}\mathcal{V} \\
&= -\int_{\mathcal{V}} \frac{\nabla v(x,t) \phi(x, v(x,t), \nabla v(x,t))}{(c+v(x,t))^2} \mathrm{d}\mathcal{V} \\
&\quad - \int_{\partial\mathcal{V}} \frac{\phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x)}{c+v(x,t)} \mathrm{d}\mathcal{S}_{\mathcal{V}} \\
&\quad + \int_{\mathcal{V}} \frac{s(x,t)}{c+v(x,t)} \mathrm{d}\mathcal{V} \\
&\geq q(t). \qquad (96)
\end{aligned}$$

Now, integrating (96) over $[t_1, t_2]$ yields (93). □

Next, we establish a dual inequality to inequality (91) that is satisfied for our thermodynamically consistent energy flow model.

Proposition 6.2: Consider the dynamical system $\mathcal{G}$ with the power balance equation (89), (90) and assume that Axiom $ii)'$ holds. Then, for every initial energy density distribution $v_0(\cdot) \in \mathcal{X}$, $t_{\mathrm{f}} \geq t_0$, and $s(t)$, $t \in [t_0, t_{\mathrm{f}}]$, such that $v_{t_{\mathrm{f}}}(x) \equiv v_0(x)$,

$$\begin{aligned}
&\int_{t_0}^{t_{\mathrm{f}}} \int_{\mathcal{V}} v(x,t) s(x,t) \mathrm{d}\mathcal{V}\mathrm{d}t \\
&\qquad - \int_{t_0}^{t_{\mathrm{f}}} \int_{\partial\mathcal{V}} v(x,t) \phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x) \mathrm{d}\mathcal{S}_{\mathcal{V}}\mathrm{d}t \\
&\geq 0, \qquad (97)
\end{aligned}$$

where $v(x,t)$, $x \in \mathcal{V}, t \geq t_0$, is the solution to (89), (90).

Proof. It follows from the Green-Gauss theorem and Axiom $ii)'$ that

$$\begin{aligned}
&\int_{t_0}^{t_{\mathrm{f}}} \int_{\mathcal{V}} v(x,t) s(x,t) \mathrm{d}\mathcal{V}\mathrm{d}t \\
&\qquad - \int_{t_0}^{t_{\mathrm{f}}} \int_{\partial\mathcal{V}} v(x,t) \phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x) \mathrm{d}\mathcal{S}_{\mathcal{V}}\mathrm{d}t \\
&= \int_{t_0}^{t_{\mathrm{f}}} \int_{\mathcal{V}} v(x,t) \frac{\partial v(x,t)}{\partial t} \mathrm{d}\mathcal{V}\mathrm{d}t \\
&\qquad + \int_{t_0}^{t_{\mathrm{f}}} \int_{\mathcal{V}} v(x,t) \nabla \cdot \phi(x, v(x,t), \nabla v(x,t)) \mathrm{d}\mathcal{V}\mathrm{d}t \\
&\qquad - \int_{t_0}^{t_{\mathrm{f}}} \int_{\partial\mathcal{V}} v(x,t) \phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x) \mathrm{d}\mathcal{S}_{\mathcal{V}}\mathrm{d}t \\
&= \int_{\mathcal{V}} \left[\tfrac{1}{2} v^2(x, t_{\mathrm{f}}) - \tfrac{1}{2} v_0^2(x) \right] \mathrm{d}\mathcal{V}
\end{aligned}$$

$$
\begin{aligned}
&+\int_{t_0}^{t_f}\int_{\partial\mathcal{V}} v(x,t)\phi(x,v(x,t),\nabla v(x,t))\cdot\hat{n}(x)\mathrm{d}\mathcal{S}_{\mathcal{V}}\mathrm{d}t \\
&-\int_{t_0}^{t_f}\int_{\mathcal{V}} \nabla v(x,t)\phi(x,v(x,t),\nabla v(x,t))\mathrm{d}\mathcal{V}\mathrm{d}t \\
&-\int_{t_0}^{t_f}\int_{\partial\mathcal{V}} v(x,t)\phi(x,v(x,t),\nabla v(x,t))\cdot\hat{n}(x)\mathrm{d}\mathcal{S}_{\mathcal{V}}\mathrm{d}t \\
&=-\int_{t_0}^{t_f}\int_{\mathcal{V}} \nabla v(x,t)\phi(x,v(x,t),\nabla v(x,t))\mathrm{d}\mathcal{V}\mathrm{d}t \\
&\geq 0, \qquad (98)
\end{aligned}
$$

which proves the result. □

Definition 6.2: For the dynamical system $\mathcal{G}$ with the power balance equation (89), (90), the function $\mathcal{E}:\mathcal{X}\to\mathbb{R}$ satisfying

$$
\mathcal{E}(v_{t_2}) \leq \mathcal{E}(v_{t_1}) + \mathcal{V}_{\mathrm{vol}}\int_{t_1}^{t_2}\hat{q}(t)\mathrm{d}t, \qquad (99)
$$

for all $s(t)$, $t\geq t_0$, and $t_2\geq t_1\geq t_0$, where

$$
\begin{aligned}
\hat{q}(t) \triangleq& \int_{\mathcal{V}} v(x,t)s(x,t)\mathrm{d}\mathcal{V} \\
&-\int_{\partial\mathcal{V}} v(x,t)\phi(x,v(x,t),\nabla v(x,t))\cdot\hat{n}(x)\mathrm{d}\mathcal{S}_{\mathcal{V}}, \qquad (100)
\end{aligned}
$$

is called the *ectropy* of $\mathcal{G}$.

Theorem 6.2: Consider the dynamical system $\mathcal{G}$ with the power balance equation (89), (90) and assume that Axiom $ii)'$ holds. Then the function $\mathcal{E}:\mathcal{X}\to\mathbb{R}$ given by

$$
\mathcal{E}(v_t) = \frac{\mathcal{V}_{\mathrm{vol}}}{2}\int_{\mathcal{V}} v_t^2(x)\mathrm{d}\mathcal{V}, \qquad (101)
$$

is an ectropy function for $\mathcal{G}$.

Proof. It follows from the Green-Gauss theorem, Axiom $ii)'$, (90), and (101) that

$$
\begin{aligned}
\dot{\mathcal{E}}(v_t) =& \mathcal{V}_{\mathrm{vol}}\int_{\mathcal{V}} v(x,t)\frac{\partial v(x,t)}{\partial t}\mathrm{d}\mathcal{V} \\
&=-\mathcal{V}_{\mathrm{vol}}\int_{\mathcal{V}} v(x,t)\nabla\cdot\phi(x,v(x,t),\nabla v(x,t))\mathrm{d}\mathcal{V} \\
&\quad+\mathcal{V}_{\mathrm{vol}}\int_{\mathcal{V}} v(x,t)s(x,t)\mathrm{d}\mathcal{V} \\
&=-\mathcal{V}_{\mathrm{vol}}\int_{\partial\mathcal{V}} v(x,t)\phi(x,v(x,t),\nabla v(x,t))\cdot\hat{n}(x)\mathrm{d}\mathcal{S}_{\mathcal{V}} \\
&\quad+\mathcal{V}_{\mathrm{vol}}\int_{\mathcal{V}} \nabla v(x,t)\phi(x,v(x,t),\nabla v(x,t))\mathrm{d}\mathcal{V} \\
&\quad+\mathcal{V}_{\mathrm{vol}}\int_{\mathcal{V}} v(x,t)s(x,t)\mathrm{d}\mathcal{V} \\
&\leq \mathcal{V}_{\mathrm{vol}}\hat{q}(t). \qquad (102)
\end{aligned}
$$

Now, integrating (102) over $[t_1,t_2]$ yields (99). □

Inequality (93) is precisely Clausius' inequality for reversible and irreversible thermodynamics as applied to infinite dimensional systems; while inequality (99) is an anti Clausius inequality that shows that a thermodynamically consistent infinite dimensional dynamical system is dissipative with storage function corresponding to the system ectropy. In addition, note that it follows from (93) that infinitesimal increment in the entropy of $\mathcal{G}$ over the infinitesimal time interval $\mathrm{d}t$ satisfies

$$
\begin{aligned}
\mathrm{d}\mathcal{S}(v_t) \geq& \left[\int_{\mathcal{V}}\frac{s(x,t)}{c+v(x,t)}\mathrm{d}\mathcal{V}\right]\mathrm{d}t \\
&-\left[\int_{\partial\mathcal{V}}\frac{\phi(x,v(x,t),\nabla v(x,t))\cdot\hat{n}(x)}{c+v(x,t)}\mathrm{d}\mathcal{S}_{\mathcal{V}}\right]\mathrm{d}t, \qquad (103)
\end{aligned}
$$

where the shifted energy density $c+v_t(x)$ plays the role of (absolute) temperature at the spatial coordinate x and time t. For an isolated dynamical system $\mathcal{G}$; that is, $s(x,t)\equiv 0$ and $\phi(x,v(x,t),\nabla v(x,t))\cdot\hat{n}(x)\equiv 0$, $x\in\partial\mathcal{V}$, (93) and (99) yield the fundamental inequalities

$$
\mathcal{S}(v_{t_2}) \geq \mathcal{S}(v_{t_1}), \quad t_2\geq t_1, \qquad (104)
$$

and

$$
\mathcal{E}(v_{t_2}) \leq \mathcal{E}(v_{t_1}), \quad t_2\geq t_1. \qquad (105)
$$

Hence, for an isolated infinite dimensional system $\mathcal{G}$ the entropy increases if and only if the ectropy decreases. It is important to note that (105) also holds in the case where $\phi(x,v(x,t),\nabla v(x,t))\cdot\hat{n}(x)\not\equiv 0$, $x\in\partial\mathcal{V}$, whereas (104) does not necessarily hold in that case.

The next theorem shows that the infinite dimensional thermodynamic energy flow model has convergent flows to Lyapunov stable uniform equilibrium energy density distributions determined by the system initial energy density distribution. However, since our continuous dynamical system $\mathcal{G}$ is defined on the infinite dimensional space $\mathcal{X}$, bounded orbits of $\mathcal{G}$ may not lie in a compact subset of $\mathcal{X}$ which is crucial to being able to invoke the invariance principle for infinite dimensional dynamical systems [46]. This is in contrast to the dynamical system $\mathcal{G}$ considered in the previous sections arising from a power balance (ordinary differential) equation defined on a finite dimensional space $\overline{\mathbb{R}}_+^q$ wherein local boundedness of an orbit of $\mathcal{G}$ ensures that the orbit belongs to a compact subset of $\overline{\mathbb{R}}_+^q$. Hence, to ensure that bounded orbits of $\mathcal{G}$ lie in compact sets we construct a larger space $\mathcal{H}\supset\mathcal{X}$ as a Sobolev space so that by the Sobolev embedding theorem [47], [48] there exists a Banach space $\mathcal{B}\supset\mathcal{H}$ such that the unit ball in $\mathcal{H}$ belongs to a compact set in $\mathcal{B}$; that is, $\mathcal{H}$ is *compactly embedded* in $\mathcal{B}$. In this case, it follows from Lemma 3 of [46] that a bounded orbit of the dynamical system $\mathcal{G}$ defined on $\mathcal{H}$ has a nonempty compact, connected invariant omega limit set in $\mathcal{B}$. For the next result, the L_2 operator norm $\|\cdot\|_{\mathrm{L}_2}$ on $\mathcal{X}$ is used for the definitions of Lyapunov, semi, and asymptotic stability. Furthermore, we introduce the Sobolev spaces $\mathcal{W}_2^1(\mathcal{V})\triangleq\{v_t:\mathcal{V}\to\mathbb{R}: v_t\in \mathrm{C}^1(\mathcal{V})\cap\mathrm{L}_2(\mathcal{V}), (\nabla v_t)^{\mathrm{T}}\in\mathrm{L}_2(\mathcal{V})\}_{\mathrm{co}}$ and $\mathcal{W}_2^0(\mathcal{V})\triangleq\{v_t:\mathcal{V}\to\mathbb{R}: v_t\in\mathrm{C}^0(\mathcal{V})\cap\mathrm{L}_2(\mathcal{V})\}_{\mathrm{co}}\equiv\mathrm{L}_2(\mathcal{V})$, where $\{\cdot\}_{\mathrm{co}}$ denotes completion of $\{\cdot\}$ in L_2 in the sense of [48], with norms

$$
\|v_t\|_{\mathcal{W}_2^1} \triangleq \left[\int_{\mathcal{V}}\left(v_t^2(x)+\nabla v_t(x)\left(\nabla v_t(x)\right)^{\mathrm{T}}\right)\mathrm{d}\mathcal{V}\right]^{\frac{1}{2}}, \qquad (106)
$$

$$
\|v_t\|_{\mathcal{W}_2^0} \triangleq \|v_t\|_{\mathrm{L}_2} = \left[\int_{\mathcal{V}} v_t^2(x)\mathrm{d}\mathcal{V}\right]^{\frac{1}{2}}, \qquad (107)
$$

defined on $\mathcal{W}_2^1(\mathcal{V})$ and $\mathcal{W}_2^0(\mathcal{V})$, respectively, where the gradient $\nabla v_t(x)$ in (106) is interpreted in the sense of a generalized gradient [48]. Note that since the solutions to (89), (90) are assumed to be two-times continuously differentiable functions on a compact set $\mathcal{V}$, it follows that $v_t(x)$, $t \geq t_0$, belongs to both $\mathcal{W}_2^1(\mathcal{V})$ and $\mathcal{W}_2^0(\mathcal{V})$.

Theorem 6.3: Consider the dynamical system $\mathcal{G}$ with power balance equation (89), (90) with $s(x,t) \equiv 0$ and $\phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x) \equiv 0$, $x \in \partial\mathcal{V}$. Assume that Axioms $i)'$, $ii)'$ hold and

$$\nabla^2 v_t(x) \nabla \cdot \phi(x, v_t(x), \frac{\partial}{\partial x} v_t(x)) \leq 0, \quad x \in \mathcal{V}, \quad v_t \in \mathcal{W}_2^1(\mathcal{V}), \quad (108)$$

where $\nabla^2 \triangleq \nabla \cdot \nabla$ denotes the Laplacian operator. Then for every $\alpha \geq 0$, $v(x,t) \equiv \alpha$ is a semistable equilibrium state of (89), (90). Furthermore, $v(x,t) \to \frac{1}{\mathcal{V}_{\mathrm{vol}}} \int_{\mathcal{V}} v_0(x) \mathrm{d}\mathcal{V}$ as $t \to \infty$ for every initial energy density distribution $v_0(\cdot) \in \mathcal{W}_2^1(\mathcal{V})$ and every $x \in \mathcal{V}$; moreover, $\frac{1}{\mathcal{V}_{\mathrm{vol}}} \int_{\mathcal{V}} v_0(x) \mathrm{d}\mathcal{V}$ is a semistable equilibrium distribution state of (89), (90). Finally, if $s(x,t) \equiv 0$ and there exists at least one point $x_{\mathrm{p}} \in \partial\mathcal{V}$ such that $\phi(x_{\mathrm{p}}, v_t(x_{\mathrm{p}}), \nabla v_t(x_{\mathrm{p}})) \cdot \hat{n}(x_{\mathrm{p}}) > 0$ and $\phi(x_{\mathrm{p}}, v_t(x_{\mathrm{p}}), \nabla v_t(x_{\mathrm{p}})) \cdot \hat{n}(x_{\mathrm{p}}) = 0$ if and only if $v_t(x_{\mathrm{p}}) = 0$, then the zero solution $v(x,t) \equiv 0$ to (89), (90) is a globally asymptotically stable equilibrium state of (89), (90).

Proof. It follows from Axiom $i)'$ that $v(x,t) \equiv \alpha$, $\alpha \geq 0$, is an equilibrium state for (89), (90). To show Lyapunov stability of the equilibrium state $v(x,t) \equiv \alpha$ consider the system shifted ectropy $\mathcal{E}_{\mathrm{s}}(v_t) = \frac{1}{2}\int_{\mathcal{V}} (v_t(x) - \alpha)^2 \mathrm{d}\mathcal{V} = \frac{1}{2}\|v_t - \alpha\|_{\mathrm{L}_2}^2$ as a Lyapunov function candidate. Now, it follows from the Green-Gauss theorem and Axiom $ii)'$ that

$$\begin{aligned} \dot{\mathcal{E}}_{\mathrm{s}}(v_t) &= \int_{\mathcal{V}} (v(x,t) - \alpha) \frac{\partial v(x,t)}{\partial t} \mathrm{d}\mathcal{V} \\ &= -\int_{\mathcal{V}} v(x,t) \nabla \cdot \phi(x, v(x,t), \nabla v(x,t)) \mathrm{d}\mathcal{V} \\ &\quad + \alpha \int_{\mathcal{V}} \nabla \cdot \phi(x, v(x,t), \nabla v(x,t)) \mathrm{d}\mathcal{V} \\ &= \int_{\mathcal{V}} \nabla v(x,t) \phi(x, v(x,t), \nabla v(x,t)) \mathrm{d}\mathcal{V} \\ &\quad - \int_{\partial\mathcal{V}} v(x,t) \phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x) \, \mathrm{d}\mathcal{S}_{\mathcal{V}} \\ &\quad + \alpha \int_{\partial\mathcal{V}} \phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x) \, \mathrm{d}\mathcal{S}_{\mathcal{V}} \\ &= \int_{\mathcal{V}} \nabla v(x,t) \phi(x, v(x,t), \nabla v(x,t)) \mathrm{d}\mathcal{V} \\ &\leq 0, \end{aligned} \quad (109)$$

which establishes Lyapunov stability of the equilibrium state $v(x,t) \equiv \alpha$.

Next, to show semistability of this equilibrium state, consider the following (scaled) ectropy and ectropy-like Lyapunov functions

$$\mathcal{E}_0(v_t) = \|v_t\|_{\mathcal{W}_2^0}^2, \quad v_t \in \mathcal{W}_2^0(\mathcal{V}), \quad (110)$$

$$\mathcal{E}_1(v_t) = \|v_t\|_{\mathcal{W}_2^1}^2, \quad v_t \in \mathcal{W}_2^1(\mathcal{V}). \quad (111)$$

It follows from (99) with $s(x,t) \equiv 0$ that $\mathcal{E}_0(v_t)$ is a nonincreasing function of time for all $v_0(\cdot) \in \mathcal{W}_2^0(\mathcal{V})$. Furthermore, it follows from the Green-Gauss theorem and the boundary condition $\phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x) \equiv 0$, $x \in \partial\mathcal{V}$, that

$$\begin{aligned} \tfrac{1}{2}\dot{\mathcal{E}}_1(v_t) &= \int_{\mathcal{V}} v(x,t) \frac{\partial v(x,t)}{\partial t} \mathrm{d}\mathcal{V} \\ &\quad + \int_{\mathcal{V}} \nabla v(x,t) \frac{\partial}{\partial t} \left(\nabla v(x,t)\right)^{\mathrm{T}} \mathrm{d}\mathcal{V} \\ &= \int_{\mathcal{V}} \nabla v(x,t) \phi(x, v(x,t), \nabla v(x,t)) \mathrm{d}\mathcal{V} \\ &\quad - \int_{\partial\mathcal{V}} v(x,t) \phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x) \, \mathrm{d}\mathcal{S}_{\mathcal{V}} \\ &\quad + \int_{\partial\mathcal{V}} \frac{\partial v(x,t)}{\partial t} D_{\hat{n}(x)} v(x,t) \, \mathrm{d}\mathcal{S}_{\mathcal{V}} \\ &\quad + \int_{\mathcal{V}} \nabla^2 v(x,t) \nabla \cdot \phi(x, v(x,t), \nabla v(x,t)) \mathrm{d}\mathcal{V} \\ &= \int_{\mathcal{V}} \nabla v(x,t) \phi(x, v(x,t), \nabla v(x,t)) \mathrm{d}\mathcal{V} \\ &\quad + \int_{\partial\mathcal{V}} \frac{\partial v(x,t)}{\partial t} D_{\hat{n}(x)} v(x,t) \, \mathrm{d}\mathcal{S}_{\mathcal{V}} \\ &\quad + \int_{\mathcal{V}} \nabla^2 v(x,t) \nabla \cdot \phi(x, v(x,t), \nabla v(x,t)) \mathrm{d}\mathcal{V}, \end{aligned} \quad (112)$$

where $D_{\hat{n}(x)} v(x,t) \triangleq \nabla v(x,t) \hat{n}(x)$ denotes the directional derivative of $v(x,t)$ along $\hat{n}(x)$ at $x \in \partial\mathcal{V}$. Next, note that for the isolated dynamical system $\mathcal{G}$ with the boundary condition $\phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x) \equiv 0$, $x \in \partial\mathcal{V}$, it follows from Axiom $i)'$, with $\mathbf{u} = \hat{n}(x)$, that $D_{\hat{n}(x)} v(x,t) \equiv 0$, $x \in \partial\mathcal{V}$. Hence, it follows from Axiom $ii)'$, (108), and (112) that $\dot{\mathcal{E}}_1(v_t) \leq 0$, $t \geq t_0$, for any $v_0(\cdot) \in \mathcal{W}_2^1(\mathcal{V})$. Furthermore, since the functions $\mathcal{E}_1(v_t)$ and $\mathcal{E}_0(v_t)$ are nonincreasing and bounded from below by zero, it follows that $\mathcal{E}_1(v_t)$ and $\mathcal{E}_0(v_t)$ are bounded functions for every $v_0(\cdot) \in \mathcal{W}_2^1(\mathcal{V})$. This implies that the positive orbit $\gamma^+(v_0) \triangleq \{v(x,t) : x \in \mathcal{V}, t \in [t_0, \infty)\}$ of $\mathcal{G}$ is bounded in $\mathcal{W}_2^1(\mathcal{V})$ for all $v_0(\cdot) \in \mathcal{W}_2^1(\mathcal{V})$. Hence, since $\mathcal{W}_2^1(\mathcal{V})$ is compactly embedded in $\mathcal{W}_2^0(\mathcal{V})$, it follows from Sobolev's embedding theorem [47], [48] that $\gamma^+(v_0)$ is contained in a compact subset of $\mathcal{W}_2^0(\mathcal{V})$. Next, define the sets $\mathcal{D}_{\mathcal{W}_2^1} = \{v_t \in \mathcal{W}_2^1(\mathcal{V}) : \mathcal{E}_1(v_t) < \eta\}$ and $\mathcal{D}_{\mathcal{W}_2^0} = \{v_t \in \mathcal{W}_2^0(\mathcal{V}) : \mathcal{E}_0(v_t) < \eta\}$ for some arbitrary $\eta > 0$. Note that $\mathcal{D}_{\mathcal{W}_2^1}$ and $\mathcal{D}_{\mathcal{W}_2^0}$ are invariant sets with respect to the dynamical system $\mathcal{G}$. Moreover, it follows from the definition of $\mathcal{E}_1(v_t)$ and $\mathcal{E}_0(v_t)$ that $\mathcal{D}_{\mathcal{W}_2^1}$ and $\mathcal{D}_{\mathcal{W}_2^0}$ are bounded sets in $\mathcal{W}_2^1(\mathcal{V})$ and $\mathcal{W}_2^0(\mathcal{V})$, respectively. Next, let $\mathcal{R} \triangleq \{v_t \in \overline{\mathcal{D}}_{\mathcal{W}_2^0} : \dot{\mathcal{E}}_0(v_t) = 0\} = \{v_t \in \overline{\mathcal{D}}_{\mathcal{W}_2^0} : \nabla v_t(x) \phi(x, v_t(x), \nabla v_t(x)) = 0, \ x \in \mathcal{V}\}$. Now, it follows from Axioms $i)'$ and $ii)'$ that $\mathcal{R} = \{v_t \in \overline{\mathcal{D}}_{\mathcal{W}_2^0} : \nabla v_t(x) = 0, x \in \mathcal{V}\}$ or $\mathcal{R} = \{v_t \in \mathcal{W}_2^0(\mathcal{V}) : v_t(x) \equiv \sigma, 0 \leq \sigma \leq \sqrt{\frac{\eta}{\mathcal{V}_{\mathrm{vol}}}}\}$; that is, $\mathcal{R}$ is the set of uniform energy density distributions which are the equilibrium states of (89), (90). Since the set $\mathcal{R}$ consists of only the equilibrium states of (89), (90), it follows that the largest invariant set $\mathcal{M}$ contained in $\mathcal{R}$ is given by $\mathcal{M} = \mathcal{R}$. Hence, noting that $\mathcal{M}$ belongs to the set of generalized (or weak) solutions to (89), (90) defined on $\mathcal{R}$, it follows from Theorem 3 of [46] that for any initial energy density distribution $v_0(\cdot) \in \mathcal{D}_{\mathcal{W}_2^1}$, $v(x,t) \to \mathcal{M}$ as $t \to \infty$ with respect to the norm $\|\cdot\|_{\mathcal{W}_2^0}$ and hence $v(x,t) \equiv \alpha$ is a semistable equilibrium state of (89), (90).

Moreover, since $\eta > 0$ can be arbitrarily large but finite and $\mathcal{E}_1(v_t)$ is radially unbounded, the previous statement holds for all $v_0(\cdot) \in \mathcal{W}_2^1(\mathcal{V})$. Next, note that since, by the divergence theorem,

$$\begin{aligned}\int_{\mathcal{V}} \frac{\partial v(x,t)}{\partial t} \mathrm{d}\mathcal{V} &= -\int_{\mathcal{V}} \nabla \cdot \phi(x, v(x,t), \nabla v(x,t)) \mathrm{d}\mathcal{V} \\ &= -\int_{\partial\mathcal{V}} \phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x)\, \mathrm{d}\mathcal{S}_{\mathcal{V}} \\ &= 0, \end{aligned} \quad (113)$$

it follows that $\int_{\mathcal{V}} v(x,t)\mathrm{d}\mathcal{V} = \int_{\mathcal{V}} v_0(x)\mathrm{d}\mathcal{V}$, $t \geq t_0$, which implies that $v(x,t) \to \frac{1}{\mathcal{V}_{\mathrm{vol}}} \int_{\mathcal{V}} v_0(x)\mathrm{d}\mathcal{V}$ as $t \to \infty$.

Finally, we show that if $s(x,t) \equiv 0$ and there exists at least one point $x_{\mathrm{p}} \in \partial\mathcal{V}$ such that $\phi(x_{\mathrm{p}}, v_t(x_{\mathrm{p}}), \nabla v_t(x_{\mathrm{p}})) \cdot \hat{n}(x_{\mathrm{p}}) > 0$ and $\phi(x_{\mathrm{p}}, v_t(x_{\mathrm{p}}), \nabla v_t(x_{\mathrm{p}})) \cdot \hat{n}(x_{\mathrm{p}}) = 0$ if and only if $v_t(x_{\mathrm{p}}) = 0$, then the zero solution $v(x,t) \equiv 0$ to (89), (90) is a globally asymptotically stable equilibrium state. Note that it follows from the above analysis with $\alpha = 0$ that the zero solution $v(x,t) \equiv 0$ is semistable and hence a Lyapunov stable equilibrium state of (89), (90). Furthermore, it follows from Axiom $ii)'$ that if $D_{\hat{n}(x_{\mathrm{p}})} v(x_{\mathrm{p}}, t) > 0$ for $x_{\mathrm{p}} \in \partial\mathcal{V}$ and some $t \geq t_0$, then the energy density decreases at this point; that is, $\frac{\partial v(x_{\mathrm{p}},t)}{\partial t} < 0$ and $D_{\hat{n}(x_{\mathrm{p}})} v(x_{\mathrm{p}}, t) \frac{\partial v(x_{\mathrm{p}},t)}{\partial t} < 0$. Alternatively, if $D_{\hat{n}(x_{\mathrm{p}})} v(x_{\mathrm{p}}, t) < 0$, then $\frac{\partial v(x_{\mathrm{p}},t)}{\partial t} > 0$ and $D_{\hat{n}(x_{\mathrm{p}})} v(x_{\mathrm{p}}, t) \frac{\partial v(x_{\mathrm{p}},t)}{\partial t} < 0$. Thus, it follows from Axiom $ii)'$, (108), and (112) that $\mathcal{E}_1(v_t)$ is a nonincreasing function of time for all $v_0(\cdot) \in \mathcal{W}_2^1(\mathcal{V})$ and since $\mathcal{E}_1(v_t)$ is bounded from below by zero, the positive orbit $\gamma^+(v_0)$ of $\mathcal{G}$ is bounded in $\mathcal{W}_2^1(\mathcal{V})$. Hence, since $\mathcal{W}_2^1(\mathcal{V})$ is compactly embedded in $\mathcal{W}_2^0(\mathcal{V})$ it follows from Sobolev's embedding theorem [47], [48] that $\gamma^+(v_0)$ is contained in a compact subset of $\mathcal{W}_2^0(\mathcal{V})$. Next, consider the (scaled) ectropy Lyapunov function $\mathcal{E}_0(v_t)$ and note that the Lyapunov derivative is given by

$$\begin{aligned}\tfrac{1}{2}\dot{\mathcal{E}}_0(v_t) &= \int_{\mathcal{V}} v(x,t) \frac{\partial v(x,t)}{\partial t} \mathrm{d}\mathcal{V} \\ &= -\int_{\mathcal{V}} v(x,t) \nabla \cdot \phi(x, v(x,t), \nabla v(x,t)) \mathrm{d}\mathcal{V} \\ &= \int_{\mathcal{V}} \nabla v(x,t) \phi(x, v(x,t), \nabla v(x,t)) \mathrm{d}\mathcal{V} \\ &\quad - \int_{\partial\mathcal{V}} v(x,t) \phi(x, v(x,t), \nabla v(x,t)) \cdot \hat{n}(x)\, \mathrm{d}\mathcal{S}_{\mathcal{V}} \\ &\leq 0. \end{aligned} \quad (114)$$

Furthermore, let $\mathcal{R} \triangleq \{v_t \in \overline{\mathcal{D}}_{\mathcal{W}_2^0} : \dot{\mathcal{E}}_0(v_t) = 0\} = \{v_t \in \overline{\mathcal{D}}_{\mathcal{W}_2^0} : \nabla v_t(x) \phi(x, v_t(x), \nabla v_t(x)) \equiv 0,\ x \in \mathcal{V}\} \cap \{v_t \in \overline{\mathcal{D}}_{\mathcal{W}_2^0} : \phi(x, v_t(x), \nabla v_t(x)) \cdot \hat{n}(x) = 0,\ x \in \partial\mathcal{V}\}$. Now, since Axioms $i)'$ and $ii)'$ hold, $\mathcal{R} = \{v_t \in \overline{\mathcal{D}}_{\mathcal{W}_2^0} : \nabla v_t(x) = 0,\ x \in \mathcal{V}\} \cap \{v_t \in \overline{\mathcal{D}}_{\mathcal{W}_2^0} : v_t(x_{\mathrm{p}}) = 0 \text{ for some } x_{\mathrm{p}} \in \partial\mathcal{V}\} = \{0\}$ and the largest invariant set $\mathcal{M}$ contained in $\mathcal{R}$ is given by $\mathcal{M} = \{0\}$. Hence, it follows from Theorem 3 of [46] that for any initial energy density distribution $v_0(\cdot) \in \mathcal{D}_{\mathcal{W}_2^1}$, $v(x,t) \to \mathcal{M} = \{0\}$ as $t \to \infty$ with respect to the norm $\|\cdot\|_{\mathcal{W}_2^0}$ which, since $\eta > 0$ is arbitrary and $\mathcal{E}_1(v_t)$ is radially unbounded, proves global asymptotic stability of the zero equilibrium state of (89), (90). □

Remark 6.1: Condition (108) physically implies that for an energy density distribution $v_t(x)$, $x \in \mathcal{V}$, the energy flow $\phi(x, v_t(x), \nabla v_t(x))$ at $x \in \mathcal{V}$ is proportional to the energy density at this point. Note that for a linear energy flow model; that is, $\phi(x, v_t(x), \nabla v_t(x)) = -k\,[\nabla v_t(x)]^{\mathrm{T}}$, where $k > 0$ is a conductivity constant, condition (108) is automatically satisfied with $-k[\nabla^2 v_t(x)]^2 \leq 0$, $x \in \mathcal{V}$.

Finally, we give an analogous proposition to Proposition 3.7 for infinite dimensional systems.

Proposition 6.3: Consider the dynamical system $\mathcal{G}$ with power balance equation (89), (90), let $\mathcal{E} : \mathcal{X} \to \mathbb{R}$ and $\mathcal{S} : \mathcal{X} \to \mathbb{R}$ denote the ectropy and entropy of $\mathcal{G}$ and be given by (95) and (101), respectively, and define $\mathcal{D}_{\mathrm{c}} \triangleq \{v_t \in \mathcal{X} : \int_{\mathcal{V}} v_t(x)\mathrm{d}\mathcal{V} = \beta\}$, where $\beta \geq 0$. Then,

$$\arg\min_{v_t \in \mathcal{D}_{\mathrm{c}}} (\mathcal{E}(v_t)) = \arg\max_{v_t \in \mathcal{D}_{\mathrm{c}}} (\mathcal{S}(v_t)) = v_t^* = \frac{\beta}{\mathcal{V}_{\mathrm{vol}}}. \quad (115)$$

Furthermore, $\mathcal{E}_{\min} \triangleq \mathcal{E}(v_t^*) = \frac{\beta^2}{2}$ and $\mathcal{S}_{\max} \triangleq \mathcal{S}(v_t^*) = \mathcal{V}_{\mathrm{vol}}[\log_e(c + \frac{\beta}{\mathcal{V}_{\mathrm{vol}}}) - \log_e c]$.

Proof. The proof is similar to the proof of Proposition 3.7 and hence is omitted. □

We close this section by noting that the results of this section can be easily generalized to the case where the energy density at a point $x \in \mathcal{V}$ is proportional to the temperature; that is, $\hat{T}(x,t) = \beta(x) v(x,t)$, where $\hat{T}(x,t)$ is the (empirical) temperature distribution over the continuum and $\beta(x)$ is the reciprocal of the specific heat at the spatial coordinate x. In this case, analogous results to the results of Section IV can be easily derived for the infinite dimensional thermodynamic model. Finally, it is important to note that the results of this section apply to an arbitrary (not necessarily Cartisian) n-dimensional space. In particular, we could consider a coordinate transformation $y = Y(x)$, where $Y(0) = 0$ and $Y : \mathcal{V} \to \mathbb{R}^n$ is a diffeomorphism in the neighborhood of the origin, so that y is defined on the image of $\mathcal{V} \subset \mathbb{R}^n$ under Y. In this case however, the nabla and gradient operators need to be redefined appropriately.

VII. CONCLUSION

In this paper we have attempted to outline a general system theory framework for thermodynamics. The proposed macroscopic mathematical model is based on a nonlinear (finite and infinite dimensional) compartmental dynamical system model that is characterized by energy conservation laws capturing the exchange of energy between coupled macroscopic subsystems. Specifically, using a large-scale systems perspective, we developed some of the fundamental properties of irreversible thermodynamic systems involving conservation of energy, nonconservation of entropy and ectropy, and energy equipartition. This model is formulated in the language of dynamical systems and control theory and it is argued that it offers conceptual advantages for describing general thermodynamic systems.

The underlying intension of this paper has been to present one of the most useful and general physical branch of science in the language of dynamical systems theory. The laws of thermodynamics reign supreme among the laws of Nature and it is hoped that this paper will help to stimulate increased interaction between physicists and dynamical systems and control theorists. Besides the fact that irreversible thermodynamics plays a critical role in the understanding of our expanding universe, it forms the underpinning of several fundamental life science and engineering disciplines including biological, physiological, and pharmocological systems, chemical reaction systems, queuing systems, ecological systems, demographic systems, telecommunication systems, transportation systems, network systems, and power systems to cite but a few examples.

Finally, future work will involve system-theoretic formulations of microscopic theories of irreversible thermodynamics and nonequilibrium statistical mechanics and statistical quantum mechanics. The newly developed notion of ectropy proposed in this paper involving an analytical description of an objective property of matter can potentially offer a conceptual advantage over the several subjective quantum expressions for entropy proposed in the literature (e.g., Daróczy entropy, Hartley entropy, Rényi entropy, von Neumann entropy, infinite-norm entropy) involving a measure of information. An even more important benefit of the dynamical system representation of thermodynamics is the potential of developing a unified classical or quantum theory which encompasses both mechanics and thermodynamics without the need for statistical (subjective or informational) probabilities.

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