FOUR RULES OF THERMODYNAMIC MODELING REVEAL GENERAL LAWS OF NATURE. FIRST: ENERGY MUST BE DEFINED. SECOND: ENTROPY MUST BE DEFINED. THIRD: STABLE EQUILIBRIUM STATES OF LOWEST ENERGY MUST HAVE ZERO TEMPERATURE. FOURTH: NONEQUILIBRIUM DYNAMICS OF IRREVERSIBLE RELAXATION MUST BE STEEPEST ENTROPY ASCENT WITH RESPECT TO SOME METRIC IN STATE SPACE

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ABSTRACT

When Thermodynamics is understood as the science/art of constructing effective models of natural phenomena by choosing a minimal level of description capable of capturing the essential features of the physical reality of interest, the scientific community has identified a set of general rules that the model must incorporate if it aspires to be consistent with the body of known experimental evidence. Some of these rules are believed to be so general that we think of them as Laws of Nature, such as the Great Conservation Principles, whose "greatness" derives from their generality, as masterfully explained by Feynman in one of his legendary lectures [1]. Also the Second Law of Thermodynamics is universally contemplated among the great laws of Nature, although no two scientists will tell you what it is in the same way (except when they agree to coauthor a paper [2] or a book [3,4]). Our understanding of the Laws of Thermodynamics has never stopped evolving over the past two centuries. The initial focus on classical statistics and kinetic theory (Boltzmann), chemical kinetics and equilibrium (van't Hoff, Gibbs), quantum statistics (Fermi-Dirac, Bose-Einstein), near equilibrium and chemical kinetics (Onsager, Prigogine), shifted in more recent decades towards complex fluids and solids, far nonequilibrium, and small and quantum systems. On and off during this evolution, some of the basic concepts need to be revisited to adapt/extend their applicability to the new realm of phenomena of interest. Questions like "What is work?", "What is heat?" [5], and "What is entropy?" [6] have risen to a currently urgent need in the quantum (Q) communities (Q information, Q computing, Q thermal machines, Q fluctuations). For example, the First Law entails the existence of property Energy for every "system" by supporting its operational definition [4], but it can do so only for models in which the "system" is well separated from its environment. In the quantum framework this means that the effects of the environment on the system can be modelled via the dependence of the Hamiltonian operator on a set of classical control parameters. Suppose system AB (Alice&Bob as a couple) is well separated but the interaction between Alice and Bob is described by a full-fleged interaction Hamiltonian V_{AB} : then the energy of AB is defined, $H_A + H_B + V_{AB}$, but the individual energies are not. The same issue is faced when B (Bath) is the environment of A, hence, the difficulties in applying thermodynamic concepts to open systems unless the effects of the full-fleged system-bath interaction can be reduced to a description in terms of local operators such as in a Lindblad-Kraus model or a steepest-entropy-ascent (SEA) model [7]. In my talk I will argue in favour of the broad generality of the SEA principle also in terms of its relations to Onsager reciprocity near equilibrium.

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This contribution is in response to a challenge that Bernard Guy proposed to some members of the JETC community about a year ago: "it would be interesting to discuss between us on how we understand the word thermodynamics. Could each of us give his/her own definition of thermodynamics and list its basic points according to him/her in less than one page?" My quick response (here slightly edited) was: "Bernard, I am afraid that each of us (and everyone else you will ask) has his/her own definition in mind (very often evolving in time...) and we all find it difficult to word it in a precise way! ... Anyway, here is an attempt to phrase my (current) point of view: Applied Thermodynamics is the art of modeling the kinematics and the dynamics of physical systems by choosing the most appropriate level of description for the 'application of interest' and implementing/exploiting the general principles/rules/laws that any such model ought to satisfy to guarantee a fair representation of the physical reality it is meant to describe (Margenau's plane of perceptions [8]). Foundational Thermodynamics is the art of extracting/distilling/identifying such general principles/rules/laws from the successes and failures of the entire body of scientific modeling efforts to rationalize experimental observations."

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