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THERMODYNAMIC AND INFORMATION ENTROPIES: CLASSICAL AND QUANTUM MEASURES MODELS – PEDAGOGICAL SOPHISTICATED BENCHMARKING FOR IT STUDENTS**S.V. Ulyanov¹, I. Kurawaki², T. Hagiwara³, Olga Tyatyushkina⁴, Olga Ivancova⁵, Yamafuji Kazuo⁶**

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The thermodynamic and information approaches for the investigation of end-to-end IT based on the laws of classical / quantum information theory and design of robust optimal control processes in non-linear non-holonomic (in general global unstable) dynamic systems are introduced. The new type of soft computing based on genetic algorithms with the fitness function as minimum entropy production rate is presented. Control objects are considered as non-linear dynamic systems that in general case described by essentially non-linear stochastic differential equations with stochastic parameters. The algorithm for the calculation of entropy production rate in control object motion and in control systems is developed. In Part 1 (this part), the interrelation between the Lyapunov function (the measure of stochastic stability) and the entropy production rate (the physical measure of controllability) is investigated. Using this interrelation the following qualitative characteristics and important interrelations are described: stochastic dynamic stability motion (average Lyapunov function), Lyapunov exponent and Kolmogorov-Sinai entropy, the physical entropy production rates, and symmetries group representation in essentially non-linear systems as coupled oscillator models. The results of computer simulation for the study entropy-like dynamic behavior for typical Benchmarks of dynamic systems as Van der Pol, Duffing, Holmes-Rand, coupled oscillators and etc. are presented. In Parts 2 and 3 the application of this approach for the simulation of dynamic entropy-like behavior and optimal control of Benchmarks as two-links manipulator in the robot for service use, robotic unicycle and a suspension system of car under stochastic excitations are presented.

Keywords: Computational Intelligence, Entropy Production Rate, Lyapunov Stability, Entropy-Like Dynamic Behavior.

ТЕРМОДИНАМИЧЕСКАЯ И ИНФОРМАЦИОННАЯ ЭНТРОПИИ: КЛАССИЧЕСКИЕ И КВАНТОВЫЕ МОДЕЛИ ВЫЧИСЛЕНИЙ – СРАВНИТЕЛЬНЫЙ АНАЛИЗ ДЛЯ СТУДЕНТОВ ИТ-НАПРАВЛЕНИЙ

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Представлены термодинамический и информационный подходы к исследованию сквозных информационных технологий, основанные на законах квантовой теории информации и разработке робастных процессов оптимального управления в нелинейных динамически неустойчивых (в общем случае глобальных неустойчивых) динамических системах. Представлен новый тип мягких вычислений на основе генетических алгоритмов с функцией пригодности в качестве минимальной скорости производства энтропии. Объекты управления рассматриваются как нелинейные динамические системы, которые в общем случае описываются существенно нелинейными стохастическими дифференциальными уравнениями со стохастическими параметрами. Разработан алгоритм расчета скорости образования энтропии неустойчивого объекта управления и в системах управления. В Части I (в данной части) исследуется взаимосвязь между функцией Ляпунова (мера стохастической устойчивости) и скоростью производства энтропии (физическая мера управляемости). Используя эту взаимосвязь, описываются следующие качественные характеристики и важные взаимосвязи: стохастическая динамическая устойчивость движения (усредненная функция Ляпунова), показатель Ляпунова и энтропия Колмогорова-Синая, скорости образования физической энтропии и представленные групп симметрий в существенно нелинейных системах в виде модели связанных осцилляторов.

Представлены результаты компьютерного моделирования для изучения энтропийного динамического поведения для типичных эталонных показателей динамических систем, таких как Ван-дер-Пол, Даффинг, Холмс-Рэнд, связанных осцилляторов и т. д. В частях 2 и 3 описано применение этого подхода для моделирования динамического энтропийного поведения и оптимального управления эталонами в качестве двухзвенного манипулятора в работе для служебного использования, одноколесном работе и системе подвески автомобиля при стохастических возмущениях представил.

Ключевые слова: интеллектуальные вычисления, скорость производства энтропии, устойчивость по Ляпунову, энтропийное динамическое поведение.

Introduction

The application of new knowledge-based control algorithms in advanced control theory of complex dynamic robotics systems has brought in necessity of the development of new calculation methods such as Computational Intelligence (CI). Traditional computing basic tools for CI is genetic algorithm (GA), fuzzy neural network (FNN), Fuzzy Sets theory, Evolution Programming, Qualitative Probabilistic Reasoning and etc. Application of CI in the classical control theory of complex robotics system motion has brought to two researching ways: 1) the study of stable motion; and 2) an unstable motion of complex dynamic systems.

In the first case (of stable motion) the development and design of intelligent control algorithms can be described in the structure submitted in [1]. The peculiarity of the given structure is the consideration of the control object in accordance of the fuzzy system theory as a “black box” and the study and optimization of an “input-output” relations using GA, FNN and fuzzy control (FC) for the description of the changing law of PID-controller parameters with a minimum control error. At the small uncontrollable external excitations or small change of parameters or structure of control objects such approach guarantees the robust and stable control. In a case of a global unstable dynamic control object such approach a presence robust and stable control does not guarantee on principle. For such kind of unstable dynamic control objects the development of a new intelligent robust algorithms based on knowledge about a movement of essentially non-linear unstable non-holonomic dynamic systems is necessary. An example of such kind of system is a new Benchmark as robotic unicycle etc. [1]. The structure of the development similar intelligent robust control algorithms in general form is shown in [2].

This approach was firstly presented in [2]. It was introduced the new physical measure of control quality to complex non-linear controlled objects described as non-linear dissipative models. This physical measure of control quality based on the physical law of minimum entropy production rate in intelligent control system and in dynamic behavior of complex object. The problem of the minimum entropy production rate is equivalent with the associated problem of the maximum released mechanical work as the optimal solutions of corresponding Hamilton-Jacobi-Bellman equations. In [3] it has shown that the variational fixed-end problem of the maximum work W is equivalent to the variational fixed-end problem of the minimum entropy production. In this case both optimal solutions are equivalent for the dynamic control of complex systems and the principle of minimum of entropy production guarantee the maximal released mechanical work with intelligent operations. This new physical measure of control quality we using as fitness function of GA in optimal control system design.

The introduction of physical criteria (the minimum entropy production rate) can guarantee the stability and robustness of control. This method differs from aforesaid design method in that a new intelligent global feedback in control system is introduced. The interrelation between the stability of control object (the Lyapunov function) and controllability (the entropy production rate) is used. The basic peculiarity of the given method is the necessity of model investigation for control object and the calculation of entropy production rate through the parameters of the developed model. The integration of joint systems of equations (the equations of mechanical model motion and the equations of entropy production rate) enable to use the result as the fitness function in GA as a new type of CI. In the given article (as Part 1) the general approach to the entropy definition and calculations from the movement equation of dynamic system model is described. The results of entropy-like dynamic behavior modeling of the typical Benchmarks of dynamic system are presented.

The thermodynamic approach for investigation and design of robust optimal control processes for non-linear non-holonomic (in general global unstable) dynamic systems in Parts 2 and 3 is introduced.

1. *Interrelation between Entropy Production Rate and Lyapunov Stability in Non-Linear Closed Dissipative Dynamic Systems*

One of the aims of thermodynamics is to provide a characterization of the states of macroscopic systems in terms of state depending on a limited number of observables. It is now well established that large classes of dynamic systems can present (under non-equilibrium conditions) complex behaviors associated with bifurcations culminating in some cases to deterministic chaos. A great deal of work has been devoted to the characterization of this complexity. A variety of quantities related to the dynamic, including entropy-like ones, have been introduced and have turned out to provide a rather successful description: Lyapunov exponents, Kolmogorov-Sinai entropy, and block entropies are some representative examples. The objective of the present work is to explore the possibilities of introducing entropy production-like quantities related directly to the dynamics of complex systems and to assess their status with respect to the thermodynamic entropy production.

This will be achieved by adopting a probabilistic formulation [4].

Remark 1. In mechanics of continuous media, elasticity theory and general dynamic system theory successfully used the methods and models described as irreversible processes from a standpoint of the phenomenological thermodynamics [5-9]. Different approaches are used in this case (see [5-7, 9] and references). The phenomenological thermodynamic approach to correctness analysis of differential equations was developed firstly in [6, 7] and the necessary conditions for physical realization of differential equations as mathematical models for real dynamic systems are studied. The interrelation between the time rate of the Lyapunov density with the time rate of the excess availability dissipation from a standpoint of phenomenological thermodynamics in [10] was studied. The same problems from a standpoint of statistical thermodynamics in [11-14] are discussed.

Remark 2. Analysis of relaxation processes as a complex system describing compound parts of “mechanical \oplus thermodynamic” behaviors in dynamic systems from the phenomenological thermodynamics standpoint carried out in [5]. Mechanical behavior of dynamic systems is described by the designated class of ordinary nonlinear differential equations. The thermodynamic behavior is characterized by a value of an entropy production and it is determined directly from a motion of a mechanical system. Interrelation between an entropy production and a Lyapunov function for closed nonlinear relaxation processes in the dynamic systems is introduced. Consequences of this interrelation are discussed.

The purpose of this work is to give a description of an application of the phenomenological thermodynamic approach developed in [7] for analysis of any class of the dynamic systems described by nonlinear dissipative differential equations. We investigate the interrelations between the notion of the Lyapunov function, entropy production and of the physical realization of approximate mathematical models describing an irreversible processes in closed nonlinear dynamic systems.

Thermodynamic criteria (the positive value of entropy production rate) as a physical measure for the realization of mathematical model (described a relaxation processes) is introduced. This criteria indicates the necessity to put extra (thermodynamic) limitations on the parameters of differential equations and on qualitative properties that describes the dynamic evolution systems. The correlation between the conditions of physical realization and the notion of stability, and correctness of the mathematical models for irreversible processes in a nonlinear dissipative dynamic systems are investigated.

Investigation of these processes is very important for a correctness analysis of dynamic evolution and stability motion of dynamic systems [7-9], and for description of artificial life conditions for micro robots [15]. Introduction of physical background in control processes is very important for design of optimal control processes using soft computing based on genetic algorithms with fitness function as a minimum entropy production in the motion of a dynamic system and in the control process [2].

1.1. Entropy production of the relaxation irreversible processes

From the thermodynamic standpoint it is needed to consider two cases in a mechanical behavior of dynamic systems [5,6]: 1) irreversible processes of generalized coordinates, and 2) irreversible processes of generalized forces. Consider the first case.

1.1.1. Entropy Production in Irreversible Processes of Generalized Coordinates

Let us consider a dynamic system with generalized coordinates x_k and described as the sum of a “reversible” x_k^r and a “irreversible” x_k^{ir} parts (see, Remark 3 below)

$$x_k = x_k^r + x_k^{ir}. \quad (1)$$

Let that for isothermal process ($T = const$) indicial equations can be described as the following: for reversible equilibrium parts of generalized coordinates as

$$x_k^r = \sum_j A_{kj} X_j \quad (2)$$

and for irreversible non-equilibrium parts of generalized coordinates as

$$\frac{dx_k^{ir}}{dt} = f_k(X_1, X_2, \dots, X_n, T). \quad (3)$$

We suggest that for coefficients A_{kj} in Eq. (2) and a function f_k in Eq. (3) the following relations are true

$$A_{kj} > 0, A_{kj} = A_{jk}, \quad (4)$$

$$f_k(0, 0, \dots, 0, T) = 0. \quad (5)$$

After differentiation of Eq. (1) in time and according to Eqs (3), and (4) we can obtain the following kinetic equations for the isothermal process

$$\frac{dx_k}{dt} = \sum_j A_{jk} \frac{dX_j}{dt} + f_k(X_1, \dots, X_n, T). \quad (6)$$

Entropy production according to the definition of generalized thermodynamic forces and corresponding to its generalized coordinates is equal to

$$\sigma = \frac{d_i S}{dt} = \frac{1}{T} \sum_j X_j \frac{dx_j^{ir}}{dt} = \frac{1}{T} \sum_k X_k f_k(X_1, \dots, X_n, T) > 0. \quad (7)$$

According to the second principle of thermodynamics entropy production σ connected with an irreversible process must be positive. Equation (7) is true for $T > 0$. Thus the kinetic equations (6) are true if for the functions $f_k(\dots)$ the relations (7) are true. It is a requirement of the thermodynamic criteria of physical realization of a mathematical model described as an irreversible process.

Example 1: Isothermal Relaxation Process of Generalized Forces. Consider an isothermal process of relaxation for generalized forces X_k occurs by fixed values of generalized coordinates $x_k = const$. Relaxation equations can be written as the following

$$\sum_j A_{jk} \frac{dX_j}{dt} + f_k(X_1, \dots, X_n, T) = 0. \quad (8)$$

Proposal 1: Equations (8) are described the relaxation process of generalized forces $X_i(t) \rightarrow 0$ for $t \rightarrow \infty$ iff the relation from Eq. (7) is true.

Proof. In this case the proof is equal to the statement that a zero solution of Eq. (8) is global asymptotic stability as stated in Lyapunov’s sentence. With this purpose the Lyapunov-Barbashin-Krasovskii (LBK)-

theorem [16] is used: Dynamic system $\frac{dz_i}{dt} = \varphi_i(z_1, z_2, \dots, z_n, t)$ ($i = 1, 2, \dots, n$) is asymptotically stable in the global by $\varphi_i(0, 0, \dots, 0, t) = 0$ if $\exists V$ with real value and $\forall z : 1) V(z) > 0; V(0) = 0$; and 2) $\frac{dV(z)}{dt} < 0$; and 3) $V(z) \rightarrow \infty$ for $\|z\| \rightarrow \infty$.

In this theorem the values of generalized forces X_k in moment of time t are not limited with any restrictions and $z = (z_1, z_2, \dots, z_n)$. For the relaxation system equations (8) consider a Lyapunov function as [7]

$$V = \frac{1}{2} \sum_{i,k} A_{ki} X_k X_i. \quad (9)$$

From Eq. (4) an indicial positive of quadratic form for $X_i \neq 0$ is followed. Derivative in time from Lyapunov function (9) is

$$\frac{dV}{dt} = \sum_{i,k} A_{ki} \frac{dX_i}{dt} X_k. \quad (10)$$

After multiplying Eq.(8) on X_k and summation on index i and k it follows

$$\sum_{i,k} A_{ki} \frac{dX_i}{dt} X_k + \sum_k X_k f_k(X_1, X_2, \dots, X_n, T) = 0. \quad (11)$$

Then

$$\sum_{i,k} A_{ki} \frac{dX_i}{dt} X_k = -\sum_k X_k f_k(X_1, X_2, \dots, X_n, T) < 0 \quad (12)$$

according to the thermodynamic conditions in Eq.(7). From Eq.(9) it follows that $V(0,0,\dots,0) = 0$ and $V \rightarrow \infty$ for $X_i \rightarrow \infty$. Thus, all conditions of LBK-theorem are fulfilled. Therefore, if the thermodynamic conditions (7) are true then Eqs (8) actually describe a relaxation process for generalized forces.

1.1.2. Entropy production in Irreversible Processes of Generalized Forces

Consider a thermodynamic system with generalized forces X_k that additive are summarized from “reversible” X_k^r and “irreversible” X_k^{ir} parts, i.e.,

$$X_k = X_k^r + X_k^{ir}. \quad (13)$$

Let that for isothermal process ($T = const$) an indicial equation can be written as following: *for reversible part*

$$X_k^r = \sum_i A_{ki} x_i \quad (14)$$

and *for irreversible part* of generalized forces

$$X_k^{ir} = f_k\left(\frac{dx_1}{dt}, \frac{dx_2}{dt}, \dots, \frac{dx_n}{dt}, T\right). \quad (15)$$

We suggest as in the first case that for coefficients A_{kj} in Eq. (14) and a function f_k in Eq. (15) the following relations are true

$$\sum_{i,k} A_{ki} x_k x_i > 0, \quad A_{kj} = A_{jk}, \quad (16)$$

$$f_k(0,0,\dots,0,T) = 0. \quad (16a)$$

The indicial kinetic equations for an isothermal process in this case can be written as

$$X_k = \sum_{k,i} A_{ki} x_i + f_k\left(\frac{dx_1}{dt}, \frac{dx_2}{dt}, \dots, \frac{dx_n}{dt}, T\right). \quad (17)$$

From the standpoint of thermodynamics for relaxation process when generalized forces are taken off the entropy production is

$$\frac{d_i S}{dt} = \frac{1}{T} \sum_k X_k^{ir} \frac{dx_k}{dt} = \frac{1}{T} \sum_k \frac{dx_k}{dt} f_k\left(\frac{dx_1}{dt}, \frac{dx_2}{dt}, \dots, \frac{dx_n}{dt}, T\right) > 0. \quad (18)$$

Example 2: Isothermal Relaxation Process of Generalized Coordinates. If generalized forces in Eq.(17) are taken off ($X_k = 0$) then this system admits the total relaxation of generalized coordinates. Relaxation equations in this case can be written as

$$\sum_i A_{ki} x_i + f_k\left(\frac{dx_1}{dt}, \frac{dx_2}{dt}, \dots, \frac{dx_n}{dt}, T\right) = 0. \quad (19)$$

Proposal 2: Equations (19) described relaxation process of generalized coordinates $x_i(t) \rightarrow 0$ for $t \rightarrow \infty$ iff the relation of Eq. (18) is true.

Proof. For the relaxation process (19) it is necessary that the entropy production rate (18) was positive, i.e., necessity and sufficiently the execution of the following condition

$$\sum_k \frac{dx_k}{dt} f_k\left(\frac{dx_1}{dt}, \frac{dx_2}{dt}, \dots, \frac{dx_n}{dt}, T\right) > 0. \quad (20)$$

Consider as Lyapunov function the following relation

$$V = \frac{1}{2} \sum_{i,k} A_{ki} x_k x_i. \quad (21)$$

According to the proposal about the coefficients A_{ki} and function $f_k(\cdot)$, and take into account the thermodynamic requirement (20) we can as in *Proposal 1* show that all requirements of *LBK* - theorem are executed. Therefore, if the thermodynamic conditions (20) are true then Eqs (19) are described actually as a relaxation process for generalized forces.

Particular Case. Let that in Eq.(17) be a generalized forces which can achieve any values and will remain constant: $X_k = const$. In this case the following *confirmation* is true: a generalized coordinates x_i as solutions of Eq.(17) achieve concrete values x_i^0 for $t \rightarrow \infty$. Assume that a generalized coordinates x_i in arbitrary time moment are additive summarized as any constant values x_i^0 and as a time function $\xi_i(t)$, i.e.,

$$x_i(t) = x_i^0 + \xi_i(t) \text{ and } x_i(0) = x_i^0 + \xi_i(0), \xi_i(0) = -x_i^0 \neq 0. \quad (22)$$

Taken into consideration that

$$X_k = \sum_i A_{ki} x_i^0 \quad (23)$$

then according to Eq. (22) kinetic equations (17) can be written as

$$\sum_i A_{ki} \xi_i + f_k \left(\frac{dx_1}{dt}, \frac{dx_2}{dt}, \dots, \frac{dx_n}{dt}, T \right) = 0. \quad (24)$$

Functions $f_k(\cdot)$ satisfy the thermodynamic requirements according to Eq.(20) as

$$\sum_k \frac{d\xi_k}{dt} f_k \left(\frac{d\xi_1}{dt}, \frac{d\xi_2}{dt}, \dots, \frac{d\xi_n}{dt}, T \right) > 0. \quad (25)$$

For $A_{ki} = A_{ik}$ and $\sum_{i,k} A_{ki} \xi_k \xi_i > 0$ the proof same as in *Proposal 1* and the system (24) admits a total relaxation of generalized coordinates ξ_i , i.e., $\xi_i \rightarrow 0$ for $t \rightarrow \infty$. Thus the solutions of Eq.(24) for $X_k = const$ and initial values $x_k = 0$ asymptotically aspire to the solutions $x_k \rightarrow x_k^0$ for $t \rightarrow \infty$. For $t = 0$ we obtain $x_k = x_k^0 + \xi_k(0)$ and $\xi_k \rightarrow 0$ for $t \rightarrow \infty$. The confirmation is true.

Similar results are fair for more general systems as

$$X_k = F_k(x_1, x_2, \dots, x_n, T) + \Phi_k \left(\frac{dx_1}{dt}, \frac{dx_2}{dt}, \dots, \frac{dx_n}{dt}, T \right). \quad (25a)$$

Let us consider more general case as Eq. (25a).

1.1.3. Generalized Case

Let us consider the motion of the dynamic system as a relaxation process described by the generalized equation [7],

$$X_a = f_a(y, \dot{y}, T), \quad a = 1, 2, \dots, m, \quad (26)$$

where X_a are generalized forces, $y = (y_1, y_2, \dots, y_n)'$ is a vector of generalized coordinates, $\dot{y} = (\dot{y}_1, \dots, \dot{y}_n)'$ is a vector of generalized velocities, T is a temperature.

In Eq. (26) we suppose that a vector - function $f_a(\dots)$ is an *analytical* function and admits the expansion in an absolutely convergence power series. In such an event

$$\begin{aligned} f_a(y, \dot{y}, T) = & \alpha_0^a + \sum_i \alpha_i^a y_i + \sum_{i,k} \alpha_{ik}^a y_i y_k + \sum_{i,k,p} \alpha_{ikp}^a y_i y_k y_p + \dots + \sum_i \beta_i^a \dot{y}_i + \sum_{i,k} \beta_{ik}^a \dot{y}_i y_k + \\ & \dots + \sum_{i,k,p} \gamma_{ikp}^a \dot{y}_i \dot{y}_k y_p + \dots \end{aligned} \quad (27)$$

On this assumption the expansion in Eq. (27) is an absolutely convergence power series. Introduce any designations:

$$F_a(y, T) = \alpha_0^a + \sum_i \alpha_i^a y_i + \sum_{i,k} \alpha_{ik}^a y_i y_k + \dots, \quad (28)$$

$$\psi_a(y, \dot{y}, T) = \sum_i \beta_i^a \dot{y}_i + \sum_{i,k} \beta_{ik}^a \dot{y}_i y_k + \dots \quad (28a)$$

Obviously that $\psi_a(y, 0, T) = 0$.

We can transform Eq. (26) in accordance with Eqs (28) and (28a) as

$$X_a = F_a(y, T) + \psi_a(y, \dot{y}, T). \quad (29)$$

If the system (26) has been in a state of equilibrium, then

$$X_a = F_a(y, T). \quad (30)$$

If the relation of Eq. (30) does not hold with $X_a = const$ or if $X_a = X_a(t)$, i.e., dependent from time t , then we must have much more generalized relations from Eq. (29).

One can see from Eq. (29) that a generalized thermodynamic force X_a is the additive function consisting from two parts: a “reversible” part $X_a^r = F_a(y, T)$ and an “irreversible” part $X_a^{ir} = \psi_a(y, \dot{y}, T)$. Thus, we can define the entropy production as the following,

$$\frac{dS}{dt} = \sigma = \frac{1}{T} \sum_a \psi_a(y_1, \dots, y_n, \dot{y}_1, \dots, \dot{y}_n, T) \dot{y}_a > 0. \quad (31)$$

Remark 3. From Eq. (29) it follows directly the definitions (1) and (13).

Considering that $T > 0$, from Eq. (31) we get the following *thermodynamic conditions for the physical realization* of nonlinear dynamic system (29)

$$\sum_a \psi_a(y_1, \dots, y_n, \dot{y}_1, \dots, \dot{y}_n, T) \dot{y}_a > 0, \forall y_k \& \dot{y}_i. \quad (32)$$

Specifically, if the function $\psi_a(\dots)$ is a linear function, then the thermodynamic criteria (32) offers to the requirement of the positive-definite quadratic form.

It must be pointed out that the equilibrium in Eq. (29) must be able to admit the following written form

$$X_a = F_a(y, T) = \frac{\partial F(y, T)}{\partial y_a} \quad (33)$$

that it is X_a must be a potential force. In Eq. (33) the function $F(y, T)$ is a *free energy* of the system (26).

Notice that only with all of above listed thermodynamic restrictions the initial system (26) can be physically realized.

Let us consider without the restriction of a generality that $X_a = 0$. In this case we deal with the relaxation of generalized coordinates y_i and the relaxation described by the following equations:

$$F_a(y, T) + \psi_a(y, \dot{y}, T) = 0, T = const \quad (34)$$

i.e., we deal with the isothermal relaxation. The relaxation is a irreversible process and must fulfill the following equality

$$\frac{d_i S}{dt} = \frac{1}{T} \sum_a \psi_a(y, \dot{y}, T) \dot{y}_a > 0 \quad (35)$$

i.e., during the relaxation we get an increase of entropy with the decrease of entropy production rate.

1.2. Entropy-Like Dynamic Behavior of Complex Non-Linear Systems

1.2.1. The Lagrange's Approach

Let us consider the Lagrangian equations

$$\frac{d}{dt} \left(\frac{\partial \mathcal{K}}{\partial \dot{q}_i} \right) - \frac{\partial \mathcal{U}}{\partial q_i} + \frac{\partial \mathcal{Q}_i}{\partial \dot{q}_i} = F_i(t), \quad (36)$$

where $L = K - U$ is Lagrangian of the dynamic system, $K = \frac{1}{2} \sum_{i,k=1}^n a_{ik} \dot{q}_i \dot{q}_k$ is the kinetic energy, and $U = \frac{1}{2} \sum_{i,k=1}^n b_{ik} q_i q_k$ is the potential energy of dynamic system, q_i is generalized coordinate accordingly.

In linear algebra it is possible define an operator A such that $q = A\xi$ or $q_i = A_{11}\xi_1 + \dots + A_{in}\xi_n$ ($i = 1, 2, \dots, n$) and $T = \frac{1}{2} \sum_{i=1}^n a_i \dot{\xi}_i^2$; $U = \frac{1}{2} \sum_{j=1}^n b_j \xi_j^2$. From Eq. (36) we can obtain

$$\ddot{\xi}_i + f_i(\dot{\xi}_1, \dots, \dot{\xi}_n) + \omega_i^2 \xi_i = 0, (i = 1, 2, \dots, n). \quad (37)$$

The Newton's Eqs (37) include additive non-conservative forces $f_i(\dot{\xi}_1, \dots, \dot{\xi}_n)$ as a particular case of Eq. (26) and (29).

Let us consider the Lyapunov function V (for $a_i = 1$ and $b_j = \omega_j^2$) as

$$V = \frac{1}{2} \sum_{i=1}^n \dot{\xi}_i^2 + \frac{1}{2} \sum_{i=1}^n \omega_i^2 \xi_i^2 = T + U = E \quad (38)$$

and

$$\frac{dV}{dt} = \sum_{i=1}^n \dot{\xi}_i \ddot{\xi}_i + \sum_{i=1}^n \omega_i^2 \xi_i \dot{\xi}_i. \quad (39)$$

After multiplication the Eq. (37) on $\dot{\xi}_i$ and a summing up on index i from 1 to n we obtain the following equation

$$\sum_{i=1}^n \dot{\xi}_i \ddot{\xi}_i + \sum_{i=1}^n \omega_i^2 \xi_i \dot{\xi}_i = - \sum_{i=1}^n \dot{\xi}_i f_i(\dot{\xi}_1, \dots, \dot{\xi}_n). \quad (40)$$

From Eqs (39) and (40) it is follows that

$$\frac{dV}{dt} = - \sum_{i=1}^n \dot{\xi}_i f_i(\dot{\xi}_1, \dots, \dot{\xi}_n) < 0. \quad (41)$$

The entropy production rate

$$\frac{d_i S}{dt} = \frac{1}{T} \sum_{i=1}^n \dot{\xi}_i f_i(\dot{\xi}_1, \dots, \dot{\xi}_n) > 0. \quad (42)$$

From Eqs (41) and (42) we can obtain

$$\frac{dV}{dt} = - \frac{1}{T} \frac{d_i S}{dt}. \quad (43)$$

Thus, we obtain the general interrelation between the Lyapunov function (stability), the entropy production rate and the full energy of dynamic system. This interrelation is one of general relations in vibration theory of dynamic systems.

From Eq.(43) it is follow that an infringement of the thermodynamic criteria of physical realization in right side of Eq. (43) an inclination for the instability of dynamic system and vice versa.

Example 3: Let us consider the dynamic system as

$$\ddot{q} + \phi(q) + \varphi(q, \dot{q}) = 0, \quad \varphi(0, \dot{q}) = \phi(q, 0) = 0. \quad (44)$$

According to the thermodynamic criteria

$$\frac{1}{T} \frac{d_i S}{dt} = \varphi(q, \dot{q}) \dot{q} > 0.$$

For particular case of Eq. (43)

$$\ddot{q} + \beta \dot{q} + \omega^2 q = 0, \quad \frac{1}{T} \frac{d_i S}{dt} = \beta \dot{q} \dot{q} = \beta \dot{q}^2$$

and a coefficient β must be positive ($\beta > 0$).

For the dynamic system

$$\ddot{q} + \beta \dot{q}^n q^m + \omega^2 q = 0, \quad \frac{1}{T} \frac{d_i S}{dt} = \beta \dot{q}^{n+1} q^m$$

and for $n=1, m=2$, $\beta > 0$, we have $\beta \dot{q}^2 q^2 > 0$. For $m=2i$ it is necessary $n=2i+1$; $\beta > 0$, $(i=1, 2, \dots, l)$.

In [7, 8] the similar interrelations between the entropy production rate and the correctness of dynamic systems are described.

Example 4: Entropy-like Values and Criteria of Dynamic Accuracy in Non-Linear Automatic Control Systems (The Accuracy of Linear Approximation). Let us consider a criteria of dynamic accuracy in non-linear automatic control system described as non-linear equations

$$\dot{x}_1 = \sum_{j=1}^n a_{ij} x_j + \Phi(x_1) + f(t); \quad |f(t)| \leq F_0$$

$$\dot{x}_i = \sum_{j=1}^n a_{ij} x_j, \quad (i \neq 1) \quad (45)$$

and a linear approximation as

$$\dot{x}_1 = \sum_{j=1}^n a_{ij} x_j + a_1 x_1 + f(t); \quad |f(t)| \leq F_0, \quad a_{10} \leq a_1 \leq a_{20}$$

$$\dot{x}_i = \sum_{j=1}^n a_{ij} x_j, \quad (i \neq 1). \quad (46)$$

An excitation $f(t)$ is a module bounded function and for $f(t)=0$ the system (46) is an asymptotically stable. The necessary and sufficient conditions for linear approximation as Eq. (46) are described in [8] as

$$\frac{dV_N}{dt} - \frac{dV_L}{dt} < 0, \quad (47)$$

where V_N and V_L are Lyapunov functions for non-linear and linear systems corresponding. From the relation of Eq. (43) and Eq. (47) follows

$$\frac{d_i S_L}{dt} - \frac{d_i S_N}{dt} < 0. \quad (48)$$

The Eq.(48) described the entropy-like criteria of dynamic accuracy in linear approximation (46) of non-linear automatic control system (45). It means that the entropy production rate in linear approximation system must be less the in non-linear system.

This approach was used in [7,8] for the description of sensitivity and invariant conditions in non-linear automatic dynamic control connected with the investigation of problems as excitation accumulations and stability on the part of generalized coordinates of dynamic systems.

1.2.2. The Hamilton's Approach (Symplectic Geometry)

The resulting unifies classical mechanics and thermodynamics. From mathematical stand point it is possible postulate that the set of all states of a thermodynamical system is a differentiable manifold M and of the finite dimension. The evolution of the closed dynamic system is defined by a semi-flow $U: R_+ \times M \rightarrow M$ generated by the vector-field $Z(e) = \frac{d}{dt}U(t, e)|_{t=0}$, $e \in M$. The vector-field does not depend explicitly on time, which means that the system is autonomous, or equivalently, is closed. The dynamical system must satisfy the two principles of thermodynamics. There exists an energy state function $H: M \rightarrow R$, such that $Z \lrcorner dH = 0$, where \lrcorner is the operator of inner product. This is only a restatement of the conservation of energy principle. In the atlas of the manifold M there exist coordinate systems in which the state functions are naturally divided in two classes: geometrical and non-geometrical state functions. To the first class belongs for example state function such as the position or the velocity of a point particle, and the second one contains for example the energy or the temperature of the system. The essential difference between a thermodynamical and mechanical systems is that the last one can be fully described without using non-geometrical state functions. The system is simple if, for each choice of the special coordinate systems, the class of it's non-geometrical state functions contains only one elements [17]. We choice the temperature as the unique non-geometrical state variable and study the systems with positive temperature T , hence $M = M \times R_+ = \{m, T\}$, $T > 0$. For simple system only one non-geometrical state variable is necessary in order to describe all the non-geometrical internal phenomena.

In this case the second principle of the thermodynamics can be formulate as following: if the system adiabatically closed then there exist a non-geometrical state function $S: M \rightarrow R$, the entropy, such that:

1) $\frac{\partial H}{\partial S} > 0$; and 2) $Z_i \lrcorner dS = \dot{S}_i \geq 0$. We cannot recover entirely the work put into the system because a part of it is always wasted by friction. The expression of S which satisfies the third principle of thermodynamics ($S(m,0) = 0$) $S(m, T) = \int_0^T \frac{1}{T} \frac{\partial H}{\partial \alpha} dT$. The vector-field $Z = (X, \dot{S})$ of a simple system will be defined in such

a way that the two principles of thermodynamics will be respected. We will always use the entropy as the non-geometrical state variable.

The first law for a closed simple system reduce to $Z \lrcorner dH = X \lrcorner dH + T\dot{S} = 0$. Hence $\dot{S} = -\frac{1}{T} X \lrcorner dH$ (see, Eq. (43)). The second law imposes $\dot{S} \geq 0$. In order to satisfy this inequality, we will adopted the Onsager's hypothesis by setting $\dot{S} = \frac{1}{T} \Lambda_s(X, X)$, where $\Lambda_s(X, X)$ is a positive semi-definite symmetric (s) quadratic form. Consequently, we have $X \lrcorner dH = -\Lambda_s(X, X)$. We can postulate that the field X is defined by $dH = -\Lambda(X)$, where $\Lambda: M \rightarrow (TM)_2^0$ is bilinear form on TM . A vector-field of $T_{(m,T)}M$ is given by a couple $X = (X_1, x_0)$, where $X_1 \in T_m M$ and $x_0 \in R$. The decomposition $df = \mathbf{d}f + \frac{\partial f}{\partial T} dT$ is used and therefore $X \lrcorner ddf = X_1 \lrcorner df + \frac{\partial f}{\partial T} x_0$. A bilinear form Λ can always be decoupled in a sum of a symmetric and anti-symmetric form, i.e., $\Lambda = \Lambda_s + \Lambda_a$, and indeed $\dot{S} = \frac{1}{T} \Lambda(X, X) = \frac{1}{T} \{ \Lambda_s(X, X) + \Lambda_a(X, X) \} = \frac{1}{T} \Lambda_s(X, X)$. Equation $\dot{S} = \frac{1}{T} \Lambda_s(X, X)$ and $dH = -\Lambda(X)$ define completely the vector-field Z that as we wished the two principles.

In the field of symplectic mechanics, where the state space reduce to the sub-manifold, we know that the vector-field X is defined by $dH = -\Omega(X)$, where $\Omega(X)$ is a symplectic 2-form [18,19]. From this standpoint view, this model appears like a generalization of mechanics. Indeed the symmetric form, absent in mechanics, has been introduced to take account dissipation. If the simple system is not isolated, the vector field X_t is simply defined by $dh = -\Lambda(X) + \omega_t$, where ω_t is the work that will be defined by a differential 1-form as $\omega_t: R \times M \rightarrow T^*M$. The work ω_t can only be produced by a change in the geometrical state variables of system; this leads us to impose an essential restriction to $\omega: \forall x_o \in R, (0, x_o) \lrcorner \omega = 0$. The first principle $Z_t \lrcorner dH = X_t \lrcorner dH + T\dot{S} = X_t \lrcorner \omega_t + Q_t$ consequently gives $\dot{S} = \frac{1}{T} \Lambda_s(X, X) + \frac{1}{T} Q_t$. Hence, if $Q_t = 0$, i.e., if the system is adiabatically closed, then we recover $\dot{S} \geq 0$. Usually, the quantity $\frac{1}{T} \Lambda_s(X, X)$ is called the internal irreversibility of the system. A dissipative mechanical system is defined by the manifold $M = T^*N$, where N is the configuration manifold. The energy (Hamiltonian) and the bilinear form Λ are given

$$H(q, p, S) = K(p) + U(q, S), \quad \Lambda(q, p, S) = \Omega(p) + \Lambda_s(q, p, S), \quad (49)$$

where $K(p)$ is the kinetic energy, $U(q, S)$ is the internal energy (thermostatic energy) of the same system but in constrained equilibrium, $\Omega(p)$ is the symplectic form on T^*M [17] and $\Lambda_s(q, p, S)$ is a positive semi-defined symmetric bilinear form operating only on the vectors of T^*N .

Example 5: A damped harmonic oscillator: $M = M \times R = R^2 \times R = \{(q, p), S\}$ with $H(q, p, S) = \frac{1}{2m} p^2 + \frac{1}{2} k(S) q^2 + f(S)$, $\Lambda(q, p, S) = dq \wedge dp + \Lambda_s(q, S) dq dp$, where $m > 0$ is the mass, $k(S)$ is the spring constant, $f(S)$ is purely thermal energy and $\Lambda_s(q, S) \geq 0$ is interpreted as the friction coefficient. With the notion $Z = (\dot{q}, \dot{p}, \dot{S})$, the equation $dH = -\Lambda_s(X)$ gives

$$\frac{1}{m} p dp + k(S) q dq = -p dq + \dot{q} dp - \Lambda_s(q, S) \dot{q} dq,$$

from which $\dot{q} = \frac{1}{m} p$, $\dot{p} = -\Lambda_s(q, S) \frac{1}{m} p - k(S) q$. The equation for the entropy production rate, $\dot{S} = \frac{1}{T} \Lambda_s(X, X)$, reduces to $\frac{d_i S}{dt} = \frac{1}{m^2 T} \Lambda_s(q, S) p^2 \geq 0$.

2. Interrelations between Entropy Production Rate, Deterministic Chaos and Lyapunov Function

Suppose that in the considered domain of variable change (y, \dot{y}) just the inequality: $F > 0$. Identify in this domain the free energy F with a Lyapunov function V , i.e., $F \equiv V$.

Theorem: With above assumption the entropy production rate $\sigma = \frac{d_i S}{dt}$ in relaxation process of the system (26) and Lyapunov function V are in the following interrelation

$$\sigma = -\frac{1}{T} \frac{dV}{dt}. \quad (50)$$

Proof: According to Eq. (33) the correlation in Eq. (34) can be rewritten as

$$\frac{\partial F}{\partial y_a} + \psi_a(y, \dot{y}, T) = 0, T = const \quad (51)$$

After multiplying both parts in Eq. (51) by \dot{y}_a and summation on index “ a ” we obtain the following equation

$$\sum_a \frac{\partial F}{\partial y_a} \dot{y}_a + \psi_a(y, \dot{y}, T) \dot{y}_a = 0, T = const. \quad (52)$$

We can write

$$\frac{dV}{dt} = \frac{\partial \mathcal{N}}{\partial y_a} \dot{y}_a = \frac{\partial F}{\partial y_a} \dot{y}_a + \sum_a \psi_a(y, \dot{y}, T) \dot{y}_a = T \frac{d_i S}{dt} = T \sigma. \quad (53)$$

Therefore, Eq. (53) can be written in the following form

$$\sigma = -\frac{1}{T} \frac{dV}{dt}, \quad (54)$$

i.e., Eq. (50).

The interrelation (50) is one of generalization in the stability theory of relaxation dissipative processes.

From Eqs (7) and (12) we obtain also

$$\sigma = \frac{1}{T} \sum_k X_k f_k(X_1, \dots, X_n, T) = -\frac{1}{T} \frac{dV}{dt}. \quad (55)$$

The relation in Eq. (55) is a result of a irreversible process in relaxation of thermodynamic forces.

Remark 4. From Eqs (50) and (51) it followed that it is possible to define a production entropy rate at the expense of irreversible processes through an accordingly selected Lyapunov function. It is well known [16] that the well defined functions (wdf's) from a Lyapunov function is also Lyapunov functions. Between these wdf's it is necessary to choose wdf that satisfies the basic thermodynamic relations (50) or (55). The entropy production is a single-value function of dynamic system parameters and Eq. (50) permits us to pick out a corresponding function V from the set of Lyapunov functions. Moreover, for every differential asymptotic stable system (in Lyapunov sentence) there exists a Lyapunov function [16] and from Eq.(50) it follows that there exists also a production entropy rate caused by an irreversible process in examined system.

2.1. Interrelations between Entropy Production Rate, Deterministic Chaos, Lyapunov Exponent and Kolmogorov-Sinai Entropy

Classical mechanics is said to be chaotic (or irregular) if adjacent trajectories in a given region of phase space diverge exponentially [20, 21]. The largest lyapunov number λ describes the asymptotic rate of exponential separation $d(t)$ between two initially close trajectories at a distance $d(0)$: $\lambda = \lim_{d(0) \rightarrow 0, t \rightarrow \infty} \frac{1}{t} \ln \frac{d(t)}{d(0)}$.

A universal quantity that measures stochasticity is the Kolmogorov-Sinai (KS) entropy h , which is defined in the general case of more than one region of connected stochasticity G as [21]: $h = \int_G \left(\sum_{\lambda_+ > 0} \lambda_+(x) \right) d\mu$, where

$d\mu$ is an element of the invariant volume (measure) in G , and x stands for the canonical coordinates and momenta. In a single region of connected stochasticity the x 's are independent of x and the integral over $d\mu$ simply yields $h = \sum_{\lambda_+ > 0} \lambda_+$. In general *KS*-entropy presents the mean value of entropy production over the basin

of attractor. The KS-entropy, h , provides a measure of the rate of loss of information in predicting the future course of the trajectory and a dynamical system is said to be chaotic if h is positive definite.

For a dynamic system $\dot{x} = F(x)$, where x, F are vectors in an n -dimensional space R^n , in the neighbourhood of a given point x_0 we can write $x = x_0 + \delta x$, where $\frac{d}{dt} \delta x = M(x_0) \delta x$, $M_{ij}(x_0) = \left. \frac{\partial F}{\partial x_j} \right|_{x=x_0}$. Besides one can construct an orthogonal system $(e_0^1, e_0^2, \dots, e_0^n)$ at the point x_0 . The n -th Lyapunov exponent in R^n is defined as follows: $\lim_{t \rightarrow \infty} \frac{1}{t} \log \left| \frac{e_t^1 \wedge e_t^2 \wedge \dots \wedge e_t^n}{e_0^1 \wedge e_0^2 \wedge \dots \wedge e_0^n} \right| = \sum_{i=1}^n \lambda_i$, where operation \wedge presents a generalization of vector product upon higher dimensional vector space.

According to the Liouville's theorem

$$\frac{\partial}{\partial t} |e_t^1 \wedge e_t^2 \wedge \dots \wedge e_t^n| = \text{div} F(x_t) |e_t^1 \wedge e_t^2 \wedge \dots \wedge e_t^n|.$$

Integration of this expression gives

$$\lim_{t \rightarrow \infty} \frac{1}{t} \log \left| \frac{e_t^1 \wedge e_t^2 \wedge \dots \wedge e_t^n}{e_0^1 \wedge e_0^2 \wedge \dots \wedge e_0^n} \right| = \lim_{t \rightarrow \infty} \frac{1}{t} \int \text{div} F(x_s) ds = \int \rho \text{div} F d\Gamma = \sum_{i=1}^n \lambda_i$$

and for non-conservative dynamic system the entropy production rate is follows $\frac{dS}{dt} = \int \rho \text{div} F d\Gamma$, where the density function ρ fulfills the Liouville's equation.

Thus $\frac{dS}{dt} = \int \rho \text{div} F d\Gamma = \sum_{i=1}^n \lambda_i = \sum_{i=1}^n \lambda_i^+ + \sum_{i=1}^n \lambda_i^-$, and for entropy production rate due to irreversible process inside the system $\frac{d_i S}{dt} = \sum_{i=1}^n \lambda_i^+$.

It is plausible that the rate at which information about the system is lost is equal to the average sum of positive Lyapunov exponents: $h = \int \rho \sum_{i=1}^n \lambda_i^+ d\mu$, where $\rho(x)$ is the invariant density of the attractor. Thus,

$h = \int \rho \frac{d_i S}{dt} d\mu = \left\langle \frac{d_i S}{dt} \right\rangle$. In most cases the λ 's are independent of x so

$$h = \sum_{i=1}^n \lambda_i^+ \int \rho d\mu = \sum_{i=1}^n \lambda_i^+ \quad \text{and} \quad h = \frac{d_i S}{dt}. \tag{56}$$

Remark 5. In [22] it is shown that there is a close relationship between the entropy production of non-equilibrium thermodynamics and the KS-entropy of the dynamic system theory. In this case we have the entropy production due to irreversible processes inside the system (a role of bifurcation) $\frac{d_i S}{dt} = \sum_{k=1}^n \lambda_k^+$, where λ_k^+ is k -th positive Lyapunov exponent. For KS-entropy with a differentiable map of finite-dimensional manifold and an ergodic measure with a compact support Ruelle is showed that $h \leq \sum_j^n \lambda_j^+$. According to Eq.(50) we can write

$$\frac{d_i S}{dt} = -\frac{1}{T} \frac{dV}{dt} = \sum_{j=1}^n \lambda_j^+ \geq h. \quad (57)$$

The Eq. (57) is the generalized form description of interrelations between the thermodynamic entropy production rate, dynamic stability of deterministic chaos, Lyapunov exponents, and *KS*- entropy.

2.2. Statistical Definition of Entropy Production Rate and Symmetries of Stochastic Dynamics

The condition of instability the two basic aspects, probability and irreversibility, already, are included. This include chaos and “non-integrability” in the sense of Poincare. There exists also classes of situations where the diffusive features play an essential role (as example, the situations studied in non-equilibrium statistical mechanics). For these situations, we must then include in the fundamental description the two aspects so conspicuous on the macroscopic level, probability and irreversibility (think about bifurcation and chaos) [23]. It is by now well established that the large classes of dynamic system can present, under non-equilibrium conditions, complex behaviors associated with bifurcations culminating in some cases to deterministic chaos. A natural description of complex dissipative systems should make use of the two principle of thermodynamics: 1) the principle of conservation of energy; and 2) the principle of non-decrease of entropy.

2.2.1 Statistical Definition of Entropy Production Rate

Having mapped the dynamics into stochastic process, it is natural to inquire about the properties of information (Shannon)-like entropies [7,8]. Specifically, the one-time entropy is considered as

$$S_I = -k_B \int \rho(x, t) \ln \rho(x, t) dx, \quad (58)$$

where k_B is Boltzman constant, and $\rho(x, t)$ is the probability density function. The change of so-defined entropy, hence the time derivative of Eq. (58), the follows as

$$\frac{dS_I}{dt} = -k_B \int (1 + \ln \rho(x, t)) \left(\frac{\partial \rho(x, t)}{\partial t} \right) dx. \quad (59)$$

According to Liouville’s theorem for the phase space $\frac{d\rho}{dt} = 0$ and

$$\frac{\partial \rho}{\partial t} = \sum_{i=1}^3 \left(\frac{\partial \rho}{\partial \dot{x}_i} \frac{\partial H}{\partial x_i} - \frac{\partial \rho}{\partial x_i} \frac{\partial H}{\partial \dot{x}_i} \right). \quad (60)$$

Inserting Eq.(60) in Eq. (59), we obtain $\frac{d\rho}{dt} = 0 \Rightarrow \frac{dS_I}{dt} = 0$, i.e., the entropy change vanishes as long as

Liouville’s theorem applies for $\rho(x, \dot{x}, t)$. Liouville’s theorem for phase space does not apply if, for example, particle-particle interactions and stochastically forced continuous time dynamic system take place.

The evolution of a stochastically forced dynamic system is given by a set of coupled first-order Langevin equations of the form

$$\dot{x} = F(x, u) + \xi(t), \quad (61)$$

where x is the state vector, F is the vector-field, u is a set of control parameters, and $\xi(t)$ stands for the effect of fluctuations of external noise on the macroscopic dynamics. The effect will be modeled as an additive multi-Gaussian white noise $\langle \xi_i(t) \xi_j(t') \rangle = D_{ij} \delta(t - t')$. The structure of the covariance matrix D_{ij} (a positive definite matrix) is imposed in the case of external noise but follows from fluctuation-dissipative types of relationships in the case of thermodynamic fluctuations. The Eq. (61) define a Markovian process of

the diffusion type and induce a Kolmogorov-Fokker-Planck (FPK) equation for the evolution of the probability density function (PDF) $\rho(x, t)$ as

$$\frac{\partial \rho}{\partial t} = -\sum \frac{\partial}{\partial x_i} (F_i \rho) + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n D_{ij} \frac{\partial^2 \rho}{\partial x_i \partial x_j}. \quad (62)$$

Therefore, Eq. (59) can be rewritten as

$$\frac{dS_I}{dt} = k_B \int (1 + \ln \rho) \left\{ \sum_i \frac{\partial}{\partial x_i} (F_i \rho) - \frac{1}{2} \sum_{i,j} \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} (D_{ij} \rho) \right\} dx. \quad (63)$$

Integrating the terms on the first sum twice by parts, we obtain

$$k_B \int (1 + \ln \rho) \frac{\partial}{\partial x_i} (F_i \rho) dx = \int \rho \frac{\partial F_i}{\partial x_i} dx = \int \rho \operatorname{div} F dx = \frac{d_e S_I}{dt}. \quad (64)$$

The second term in Eq. (63) positive definite

$$\frac{d_i S_I}{dt} = \frac{1}{2} \sum_{i,j} D_{ij} \int \frac{1}{\rho} \left(\frac{\partial \rho}{\partial x_i} \right) \left(\frac{\partial \rho}{\partial x_j} \right) dx \geq 0 \quad (65)$$

and present the analogy of *Fisher information amount*.

Thus, the Eq. (64) and (65) led to identify flux and (information) entropy rate correspondingly. Away from equilibrium the entropy production rate (65) enters the entropy balance through

$$\frac{dS_I}{dt} = \frac{d_e S_I}{dt} + \frac{d_i S_I}{dt} \quad (65)$$

with $\frac{d_i S_I}{dt}$ being the entropy flow. In the absence of noise, expression (64) reduce to the sum of Lyapunov exponents as in Eq.(57) - a negative quantity for a dissipative dynamic system.

Remark 6. For a particular case of μ - space $(x, y, z, p_x, p_y, p_z, t)$ the FPK-equation is following:

$$\frac{\partial \rho}{\partial t} = -\sum \frac{\partial}{\partial p_i} (F_i(p, t) \rho) + m^2 \sum_{i=1}^n \sum_{j=1}^n \frac{\partial^2 \rho}{\partial p_i \partial p_j} (D_{ij}(p, t) \rho),$$

where m is a mass of interacting particles, $F_i(p, t)$ is the drift vector components of FPK-equation, and $D_{ij}(p, t)$ is the diffusion tensor elements. Then

$$\frac{dS_I}{dt} = k_B \int (1 + \ln \rho) \left\{ \sum_i \frac{\partial}{\partial p_i} (F_i(p, t) \rho) - m^2 \sum_{i=1}^n \sum_{j=1}^n \frac{\partial^2 \rho}{\partial p_i \partial p_j} (D_{ij}(p, t) \rho) \right\} d\tau \quad (67)$$

Integrating in Eq. (67) the terms of the first sum twice by parts

$$\int (1 + \rho) \frac{\partial}{\partial p_i} (F_i \rho) d\tau = \int \rho \frac{\partial F_i}{\partial p_i} d\tau.$$

Let us consider the Maxwell-Boltzman non-isotropic distribution

$$\rho = g(x, y, z, t) \exp \left\{ -\frac{p_x^2}{2mk_B T} - \frac{p_y^2}{2mk_B T} - \frac{p_z^2}{2mk_B T} \right\}$$

with $g(x, y, z, t)$ as the self-consistent charge density and the exponential function describing the distribution of the incoherent part of the kinetic particle energy. The coherent part of the kinetic energy eliminated since it does not cause the terms of the second sum of eq. (67) evaluate to

$$m^2 \int (1 + \ln \rho) \frac{\partial^2 \rho}{\partial p_i \partial p_j} (D_{ij}(p, t) \rho) d\tau = -\frac{m}{k_B T} \delta_{ij} \int D_{ij} \rho d\tau.$$

In summary, the change of entropy caused by a Markovian process can be expressed in terms of FPK-equation coefficient as [24]

$$\frac{dS_I}{dt} = k_B \sum_{i=1}^n \left(\left\langle \frac{\partial F_i}{\partial p_i} \right\rangle + \frac{m}{k_B T} \langle D_{ij} \rangle \right). \quad (68)$$

where $\frac{d_e S_I}{dt} = k_B \sum_{i=1}^3 \left\langle \frac{\partial F_i}{\partial p_i} \right\rangle$ and $\frac{d_i S_I}{dt} = \sum_{i=1}^3 \frac{m}{T_i} \langle D_{ij} \rangle$.

Example 6: Holmes-Rand non-linear oscillator. Consider an application of a stability analysis on the basis of the interrelation between the entropy production and Lyapunov function to a Benchmark as Holmes-Rand oscillator

$$\ddot{x} + (\alpha + \beta x^2) \dot{x} - \gamma x + x^3 = 0, \quad (69)$$

where α, β and γ are parameters. The system (69) has a close resemblance to the Duffing-van der Pol class of non-linear oscillators. In this case we get a four-parameter symmetry group [15] where the associated vector-fields and the dynamic vector field

$$X = y \frac{\partial}{\partial x} - \left[\left(\beta x^2 + \frac{4}{\beta} \right) y + x^3 + \frac{3}{\beta^2} x \right] \frac{\partial}{\partial y} \quad (70)$$

are associated with Eq. (69). From Eq.(70) follows that the dynamic system (69) has a specific symmetries for $\alpha = \frac{4}{\beta}$ and $\gamma = -\frac{3}{\beta^2}$. The integral of motion I for the Eq.(69) for the choice $\alpha = \frac{4}{\beta}$ and $\gamma = -\frac{3}{\beta^2}$ is

$$I = \exp[(3/\beta)t] \left[\dot{x} + \frac{\beta}{3} x^3 + \frac{1}{\beta} x \right] \quad (71)$$

and we end up with a first-order inhomogeneous Abel's equation:

$$\dot{x} + \frac{1}{3} \beta x^3 + \frac{1}{\beta} x = I \exp\left[-\left(\frac{3}{\beta}\right)t\right]. \quad (72)$$

The Holmes-Rand non-linear oscillator does not pass the Painleve' test as it admits a movable algebraic branch point. It has been pointed out that there exist second-order systems which are non-Painleve' but which nevertheless possess one integral of motion and hence are integrable. In this case the choice $\alpha = \frac{4}{\beta}$ and

$\gamma = -\frac{3}{\beta^2}$ of the Holmes-Rand non-linear oscillator belongs to the above category [15].

The Lyapunov function for the system (70) is described as $V = \frac{1}{2}\dot{x}^2 + U(x)$, where $U = \frac{1}{4}x^4 - \frac{1}{2}\gamma x^2$

. Entropy production rate in a system motion is $\frac{d_i S}{dt} = (\alpha + \beta x^2)\dot{x}^2$. In this case Eq.(70) can be written as

$\ddot{x} + (\alpha + \beta x^2)\dot{x} + \frac{\partial U}{\partial x} = 0$ and after multiplying the left part of this equation on \dot{x} we obtain

$(\ddot{x} + (\alpha + \beta x^2)\dot{x} + \frac{\partial U}{\partial x})\dot{x} = 0$. The value of $\frac{dV}{dt}$ calculated as $\frac{dV}{dt} = \dot{x}\ddot{x} + \frac{\partial U}{\partial x}\dot{x}$ and after a simple algebraic transformation we obtain in this case

$$\frac{dV}{dt} = -\frac{1}{T} \frac{d_i S}{dt}, \quad (73)$$

where T is a normalization factor.

From the analysis of the relations in Eqs (71) – (73) it shows that the specific symmetries of Eq. (69) for $\alpha = \frac{4}{\beta}$ and $\gamma = -\frac{3}{\beta^2}$ with the dynamic vector-field (70) produce the maximum stable non-equilibrium states with the minimum production entropy in these states.

For $\beta = 0$ from Eq. (69) we obtain the equation of motion of the force-free Duffing oscillator and for exactly the same parametric choice $2\alpha^2 = 9\gamma$ the Panleve' property holds [15] for this equation. In this case [15] the integral of motion $I = \exp[\frac{4}{3}\alpha t][\dot{x}^2 + \frac{2}{3}\alpha x\dot{x} + \frac{1}{2}x^4 + \frac{2}{9}\alpha^2 x^2]$. The relation in Eq. (73) is true with the Lyapunov function as for Holmes-Rand oscillator and $\frac{d_i S}{dt} = \alpha \dot{x}^2$.

Eqs (40) and (42) describes a generalized interrelation between Lyapunov functions V (qualitative measure of mechanical motion) and an entropy production $\frac{d_i S}{dt}$ (quantitative measure of thermodynamic behavior).

For $\alpha = -1, \beta = 1, \gamma = -1$ and without the non-linear term x^3 we obtain the result discussed in [16] for van der Pol oscillator.

3. Simulation Results of Entropy-Like Behavior of Typical Dynamic Systems

3.1. Definition of Entropy Production Rates of Benchmarks

The thermodynamic model representation of dynamic equations of motion for a control object (Plant) in a general form as closed and open dynamic systems is developed in Ref.2). Based on this, the analysis on Plant's postural stability control is done and results of computer simulation is compared.

Let us introduce results of entropy production calculation and dynamic behavior for typical systems as

1. Van der Poll Oscillator Model

$$\ddot{x} + (x^2 - 1)\dot{x} + x = 0.$$

Entropy Production

$$\frac{dS}{dt} = \frac{1}{T} (x^2 - 1) \dot{x}^2.$$

2. Duffing Oscillator Model

$$\ddot{x} + \dot{x} - x + x^3 = 0.$$

Entropy Production

$$\frac{dS}{dt} = \frac{1}{T} \dot{x}^2.$$

3. Holmes-Rand (Duffing-Van der Pol) Oscillator Model

$$\ddot{x} + (x^2 - 1)\dot{x} - x + x^3 = 0.$$

Entropy Production

$$\frac{dS}{dt} = \frac{1}{T} (x^2 - 1) \dot{x}^2.$$

4. Duffing Oscillator Model with parametric excitation of dissipative force

$$\ddot{x} + k(1 + A\sin\omega t)\dot{x} - x + x^3 = 0.$$

Entropy Production

$$\frac{dS}{dt} = \frac{k}{T} (1 + A\sin\omega t) \dot{x}^2.$$

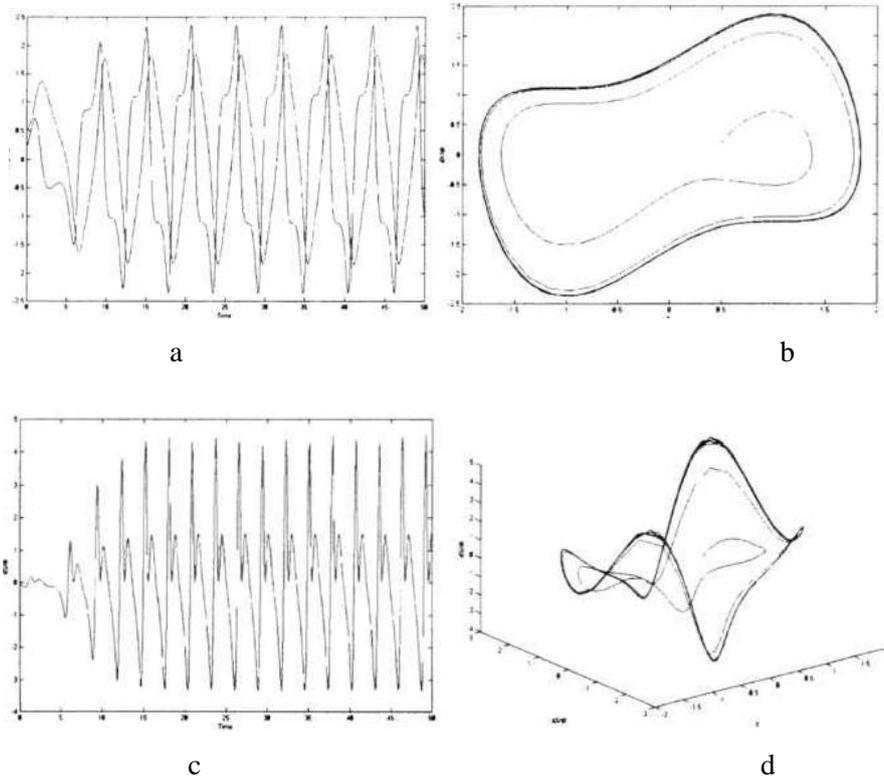


Fig. 3. Simulation results of entropy-like behavior for Holmes-Rand oscillator. a: Free motion with initial states $x_0 = 0.5$; $\dot{x}_0 = 0.2$; b: phase portrait; c: temporal entropy-like behavior (entropy production rate); d: 3D simulation entropy-like behavior.

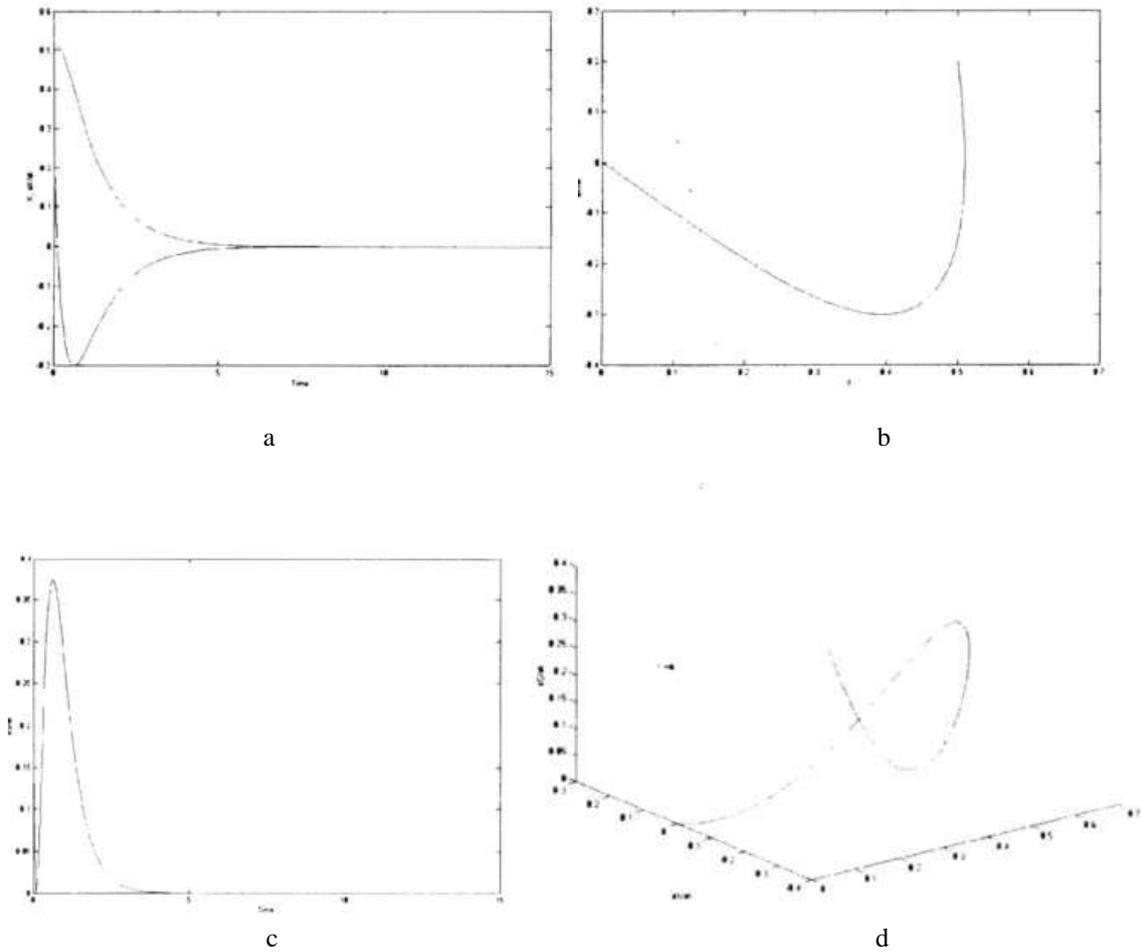


Fig. 4. Simulation results of entropy-like behavior for Holmes-Rand oscillator with symmetric – $\alpha = 4/\beta$, $\gamma = -4/\beta^2$: a: free motion with initial states $x_0 = 0.5$; $\dot{x}_0 = 0.2$; b: phase portrait; c: temporal entropy-like behavior (entropy production rate); d: 3D simulation entropy-like behavior.

$$\frac{dS}{dt} = \frac{k}{T}(1 + A\sin\omega t)x^2,$$

Also consider the Lyapunov function as

$$V = \left(\frac{x^2}{2} + \frac{\dot{y}^2}{2} + \frac{x^2}{2} + \frac{y^2}{2} + \frac{\alpha(x-y)^2}{2}\right) > 0, \tag{74}$$

In this case,

$$\frac{dV}{dt} = \dot{x}\dot{x} + \dot{y}\dot{y} + x\dot{x} + y\dot{y} + \alpha(x\dot{x} - \dot{x}y - \dot{y}x + y\dot{y}), \tag{75}$$

The dynamic system with Lyapunov function is a system of two coupled nonlinear oscillators as

$$\begin{cases} \ddot{x} + (\dot{x}^2 + x^2 - 1)\dot{x} + x + \alpha(x - y) = 0 \\ \ddot{y} + (\dot{y}^2 + y^2 - 1)\dot{y} + y + \alpha(y - x) = 0 \end{cases} \tag{76}$$

After multiplication on \dot{x} and \dot{y} in both equations of system and after simple algebraic transformations, we write final results as follows:

$$\frac{dV}{dt} + (\dot{x}^2 + x^2 - 1)\dot{x}^2 + (\dot{y}^2 + y^2 - 1)\dot{y}^2 = 0. \tag{77}$$

From Eq. (77), it follows

$$\frac{dV}{dt} = \sum_{i=1}^2 \frac{d_i S}{dt} \tag{78}$$

From Eq. (78), we get the law on additive properties of entropy production in dynamic systems.

In a more complex case as

$$V = \left(\frac{\dot{x}^2}{2} + \frac{\dot{y}^2}{2} + \frac{\dot{z}^2}{2} + \frac{x^2}{2} + \frac{y^2}{2} + \frac{z^2}{2} + \frac{\alpha(|x-y|-z)^2}{2} \right),$$

we have

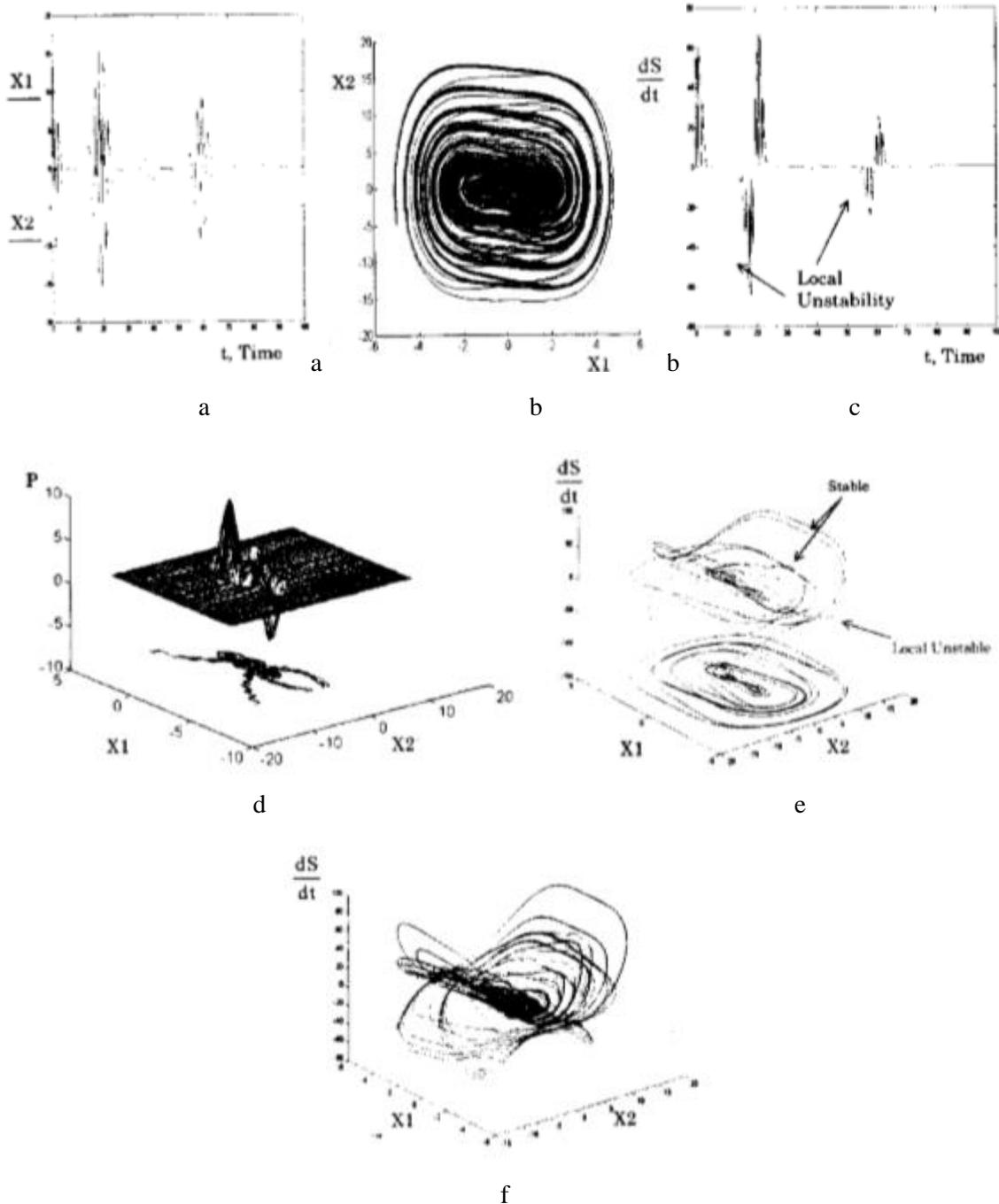


Fig. 5. Entropy analysis of stability on nonlinear parametric dissipative Duffing oscillator: a: temporal behavior of oscillator with initial states $x_0 = -1,75$, $\dot{x}_a = -1$, $\omega = 0,1$; b: the phase portrait; c: temporal entropy-like behavior with local unstable states; d: power distribution; e: 3D simulation of entropy-like behavior with one unstable state; f: 3D simulation of entropy-like behavior with n unstable states.

$$\begin{cases} \dot{x} + (\dot{x}^2 + x^2 - 1)\dot{x} + x + \alpha(x + y - z) = 0 \\ \dot{y} + (\dot{y}^2 + y^2 - 1)\dot{y} + y + \alpha(y - x + z) = 0 \\ \dot{z} + (\dot{z}^2 + z^2 - 1)\dot{z} + z + \alpha(z - x + y) = 0 \end{cases}$$

and

$$\frac{dV}{dt} = - \sum_{i=1}^3 \frac{d_i S}{T_i dt}; \quad \frac{d_1 S}{dt} = \frac{1}{T_1} (\dot{x}^2 + x^2 - 1)\dot{x}^2; \quad \frac{d_2 S}{dt} = \frac{1}{T_2} (\dot{y}^2 + y^2 - 1)\dot{y}^2;$$

$$\frac{d_3 S}{dt} = \frac{1}{T_3} (\dot{z}^2 + z^2 - 1)\dot{z}^2,$$

for three coupled nonlinear oscillators.

Conclusions

The interrelations between the notion of the Lyapunov function (stability conditions), entropy production (thermodynamic behavior) and of the physical realization of approximate mathematical models describing an irreversible relaxation processes in closed nonlinear dissipative dynamic systems are investigated. Thermodynamic criteria (the positive value of production entropy) as a physical measure for the realization of mathematical model described a relaxation processes is introduced. This criteria indicates on the necessity to put extra (thermodynamic) limitations on the parameters of differential equations and on symmetries properties describes the evolution of nonlinear dynamic systems. Similar interrelation between Lyapunov functions and an entropy production in open dissipative dynamic systems with entropy structure exchange is needed to study.

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Appendix 1: von Neumann versus Shannon entropy

In *classical statistical thermodynamics* the entropy is defined as $S = k \log W$, where k is Boltzmann's constant and W is the number of accessible microstates consistent with the known macrostate of the system. If all the microstates are equally probable, then each has probability $p = \frac{1}{W}$. The *Boltzmann entropy* can then be written $S = -k \log p$. Alternatively, if the different microstates have differing probabilities, say p_i for the i^{th} state, then the entropy would be $-k \log p_i$ with a probability of p_i . So the ensemble average entropy would be Boltzmann entropy $S_B = -k \sum_i p_i \log p_i$. Dimensionless entropy is defined by dropping the Boltzmann constant factor. We shall assume dimensionless entropy from here on.

In *information theory*, the *Shannon entropy* (or information) is defined in the same way. Let's say a message is transmitted using symbols x_i , and that these are known to occur with probability p_i . (This may be known, for example, because past messages have shown that x_1 occurs with a relative frequency p_1 , etc.). How much information is there in a message N symbols long? Well, it is N times the average information per symbol transmitted, and the latter is defined as $S_{sh} = -\sum_i p_i \log_2 p_i$. Note that whereas entropy in physics is defined using the natural logarithm, in information theory \log_2 is used. This is natural because it means that one even binary choice corresponds to one unit of information (one bit). Some authors sometimes employ entropy defined using logs to the base of some other integer, for example the dimension of some relevant Hilbert space.

By analogy, *von Neumann* defined the entropy of a mixed quantum state as,

$$S_{vN} = -\text{Tr } \rho \log_2 \rho .$$

Consider first of all that the density matrix has been put in diagonal form with respect to an orthonormal basis, $|\phi_i\rangle$. It can always be written $\rho = \sum_i p_i |\phi_i\rangle\langle\phi_i|$ and the von Neumann entropy is then,

$$\begin{aligned} S_{vN} = -\text{Tr } \rho \log_2 \rho &= -\text{Tr} \left(\rho \sum_i \log_2 p_i |\phi_i\rangle\langle\phi_i| \right) = -\text{Tr} \left(\sum_j p_j |\phi_j\rangle\langle\phi_j| \sum_i \log_2 p_i |\phi_i\rangle\langle\phi_i| \right) \\ &= -\sum_k \langle\phi_k| \sum_j p_j |\phi_j\rangle\langle\phi_j| \sum_i \log_2 p_i |\phi_i\rangle\langle\phi_i| \phi_k\rangle = -\sum_{k,j,i} \delta_{kj} p_j \delta_{ji} \log_2 p_i \delta_{ik} \\ &= \boxed{-\sum_i p_i \log_2 p_i} \end{aligned}$$

So the von Neumann entropy is the same as the Shannon entropy in this case.

This is not surprising since we can imagine the classical message symbols, x_i , to be replaced by the quantum states $|\phi_i\rangle$. Since the latter are orthogonal they can be distinguished with certainty, as can the classical symbols, and hence there is no physical difference between the two situations.

It is important to realise that the von Neumann entropy is *zero* for any pure state. In the spectral representation of the density matrix, one p_i will be 1 and the rest zero. Note that this is true even if the pure state in question is expressed as a superposition of some basis states, e.g. $\alpha|\phi_1\rangle + \beta|\phi_2\rangle$. Of course this must be so: mathematically because we can always change basis so that $|\phi_1'\rangle = \alpha|\phi_1\rangle + \beta|\phi_2\rangle$, and physically because there is no more information to be had beyond the specification of the Hilbert state vector.

Note that the von Neumann entropy does not depend upon the basis chosen, because it depends only upon the eigenvalues of the density matrix. Thus changing basis so that $\rho \rightarrow U^\dagger \rho U$ leaves the von Neumann entropy unchanged (and recalling that bases are always related by a unitary transformation). By the same token, a quantum state changes in time by unitary evolution. Consequently unitary transformations of the form $\rho \rightarrow U^\dagger \rho U$ also represent temporal evolution, and hence the entropy is constant so long as unitary evolution applies. Quite how this is consistent with the classical concept of a relentless increase in entropy is discussed below.

The difference between von Neumann and Shannon entropy arises when we consider a mixture of quantum states which are not orthogonal. Suppose now that $\rho = \sum_i p_i |\tilde{\phi}_i\rangle\langle\tilde{\phi}_i|$, where the states $|\tilde{\phi}_i\rangle$ are *not* orthogonal. These states are therefore not distinguishable with certainty. If we ignore this fact we would once again get the Shannon entropy, Shannon $S_{Sh} = -\sum_i p_i \log_2 p_i$. But in truth the amount of information conveyed by a sequence of $|\tilde{\phi}_i\rangle$ states must be rather less than this, because of the noise caused by the lack of perfect distinguishability of the “symbols”. The von Neumann entropy properly accounts for this. An example makes this clear.

Example. Consider once again the mixture of two spin $\frac{1}{2}$ particles. One particle is in the z -up spin state, and the other in the x -up state. From the classical (Shannon) point of view, we have a mixture with $p_1 = p_2 = 0.5$, giving an entropy of $-0.5 \log_2 0.5 \times 2 = 1$. The density matrix in the z -representation is,

$$\rho = 0.5 |\uparrow\rangle\langle\downarrow| + 0.5 \times \frac{1}{\sqrt{2}} [|\uparrow\rangle + |\downarrow\rangle] = \begin{pmatrix} 0.75 & 0.25 \\ 0.25 & 0.25 \end{pmatrix}.$$

To find the von Neumann entropy we need to diagonalise the density matrix, i.e. to find its eigenvalues. This is done by solving the secular equation: $\left\| \begin{pmatrix} 0.75 - \lambda & 0.25 \\ 0.25 & 0.25 - \lambda \end{pmatrix} \right\| = 0$. This yields $\lambda = 0.1464$ or 0.8536 . The von Neumann entropy is thus,

$$S_{vN} = -0.1464 \log_2 0.1464 + 0.8536 \log_2 0.8536 = 0.6007.$$

So, only ~ 0.6 of a bit of information would be conveyed per quantum symbol transmitted in this example, compared with 1 bit per symbol in the classical Shannon case. Quite generally we find,

$$S_{vN} \leq S_{Sh}.$$

The equality holds only when the mixture is considered to consist of orthogonal quantum states. This, of course, is possible for any mixture. The von Neumann entropy does not depend upon the basis chosen. The Shannon entropy does. For a quantum mixture the Shannon entropy is just wrong.

Remark. The Shannon entropy is basis dependent and incorrect on physical grounds. But the formula $S_{vN} = -\text{Tr } \rho \log_2 \rho$ does have a degree of arbitrariness and some authors have proposed alternative definitions. However, the sub-additivity inequality (discussed below) is sufficient to imply the von Neumann formula. The sub-additivity inequality holds that, for a bipartite system, the entropy does not exceed the sum of the entropies of its parts: $S_{AB} \leq S_A + S_B$. This inequality, together with the condition that the equality hold only for uncorrelated sub-systems $AB = A \otimes B$, is claimed to yield the von Neumann formula. The inequality $S_{AB} \leq S_A + S_B$ seems to be physically motivated, so this is a strong argument in favour of the von Neumann entropy.

The von Neumann Entropy Inequalities

We have seen one already $S_{vN} \leq S_{Sh}$.

Quantum information amount (same as in classical case) is positive, i.e. $S(A:B) \geq 0$, but different from classical case when $0 \leq S(A:B) \leq \min[S(A), S(B)]$ in quantum case we have

$$0 \leq S(A:B) \leq 2 \min[S(A), S(B)].$$

This inequality follows from the definition of $S(A:B)$ and “Araki-Lieb inequality” as $|S(A) - S(B)| \leq S(A, B)$ (see below). Maximum entropy possible is $S_{vN} \leq S_{vN}^{\max} = \log_2 N$ where N is the number of non-zero eigenvalues of the density matrix. The maximum entropy is realized when there is an equal probability ($1/N$) for all the orthogonal eigenstates, i.e. maximum randomness. Within a given Hilbert space, the maximum is greatest when all states contribute, i.e. when N is the dimension of the Hilbert space.

Example: Entropy Change on Mixing – Concavity. Suppose we have several separate mixtures over the same Hilbert space, ρ_1, ρ_2, \dots , where, $\rho_1 = \sum_i p_{1i} |\phi_i\rangle\langle\phi_i|$, $\rho_2 = \sum_i p_{2i} |\phi_i\rangle\langle\phi_i|$, etc. Then we can make a new mixture by combining these mixtures in the ratios (probabilities) q_1, q_2, \dots , where $\sum_j q_j = 1$. The new mixture of mixtures is clearly, $\rho_T = \sum_j q_j \rho_j = \sum_{i,j} q_j p_{ji} |\phi_i\rangle\langle\phi_i|$. The von Neumann entropy of the mixture of mixtures will generally be greater than the average of the entropies of the constituent mixtures, i.e., $S_{vN} \rho_T = S_{vN} \left(\sum_j q_j \rho_j \right) \geq \sum_j q_j S_{vN} \rho_j$.

This is referred to as “concavity”. This inequality corresponds to the notion that information is lost on mixing. Physically this is because we have more information when we know all the quantities q_j, ρ_j , than when we know only ρ_T . Knowing only ρ_T we cannot re-create the original q_j, ρ_j , because there are obviously many ways the total ρ_T can be decomposed into sub-mixtures. Thus, information has been *lost* and the entropy *increases*. In other words, the less we know about how the final mixture was prepared, the greater the entropy. The equality is achieved iff all the sub-mixture density matrices are the same.

Remark. Do not confuse a mixture, in this sense, with physically mixing two or more systems. The latter really means adding systems together. In contrast, in a statistical mixture we still have just one system, but we don’t know for sure which one it is. Thus, physically mixing systems is an AND operation, whereas a quantum mixture is an OR operation.

Example. Consider just two sub-mixtures with density matrices, $\begin{pmatrix} 0.75 & 0 \\ 0 & 0.25 \end{pmatrix}$ and $\begin{pmatrix} 0.125 & 0 \\ 0 & 0.875 \end{pmatrix}$. The von Neumann entropies of these are respectively $-0.75 \log_2 0.75 + 0.25 \log_2 0.25 = 0.8113$ and $-0.125 \log_2 0.125 + 0.875 \log_2 0.875 = 0.5436$. Suppose these are combined 50% / 50%, then the average entropy before mixing is $0.5 (0.8113 + 0.5436) = 0.6774$.

The mixture of mixtures has density matrix $\begin{pmatrix} 0.5 & 0.75 + 0.125 & 0 \\ 0 & 0.5 & 0.25 + 0.875 \end{pmatrix}$ and this has von Neumann entropy $-0.4375 \log_2 0.4375 + 0.5625 \log_2 0.5625 = 0.9887$. Hence, the mixture of mixtures has a larger entropy than the original average entropy ($0.9887 > 0.6774$).

Combined States – Subadditivity

The notion of “combined states” should not be confused with mixing sub-mixtures. Pure quantum states might be composed of two parts. For example, we may be considering deuterons, and each of the pure quantum states of a given deuteron might be considered as a combined state of a proton and a neutron. The simplest

Hilbert space of combined states is the direct product of the constituent spaces: $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. In this case the A and B states are uncorrelated, i.e., given a state of the A component there is no preference for any particular B state. In this case the von Neumann entropy displays its “extensive” nature, i.e., the total entropy is just the sum of the entropies of the component sub-states, for $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$: $S_{vN}^{AB} = S_{vN}^A + S_{vN}^B$. This is obvious because the probability of the combined state i of A and j of B is clearly just $p_i^A p_j^B$, and hence,

$$\begin{aligned} S_{vN}^{AB} &= -\sum_{i,j} p_i^A p_j^B \log_2 p_i^A p_j^B = -\sum_{i,j} p_i^A p_j^B \log_2 p_i^A + \log_2 p_j^B \\ &= -\sum_{i,j} p_i^A p_j^B \log_2 p_i^A - \sum_{i,j} p_i^A p_j^B \log_2 p_j^B = -\sum_i p_i^A \log_2 p_i^A - \sum_j p_j^B \log_2 p_j^B \\ &= [S_{vN}^A + S_{vN}^B]. \end{aligned}$$

But what happens if we confine the combined state Hilbert space to some sub-set of the product space, i.e., $\mathcal{H} \subset \mathcal{H}_A \otimes \mathcal{H}_B$. For example, a deuteron must be a spin 1 combination of a proton and a neutron, since the singlet spin state is not bound by the strong nuclear force. This means there are now correlations between the components states. In our deuteron example the spin states of the proton and neutron are correlated. There are therefore fewer states available to the combined system than were available in the product space $\mathcal{H}_A \otimes \mathcal{H}_B$. Thus we therefore expect, for $\mathcal{H} \subset \mathcal{H}_A \otimes \mathcal{H}_B$: $S_{vN}^{AB} \leq S_{vN}^A + S_{vN}^B$ with equality holding only when $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Physically, the correlations present within H create a degree of order, and hence reduce the entropy. Inequality $S_{vN}^{AB} \leq S_{vN}^A + S_{vN}^B$ is known as subadditivity. Equality holds iff $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ with no correlations between the two parts.

Combined States - The Triangle Inequality & Entanglement

Inequality $S_{vN}^{AB} \leq S_{vN}^A + S_{vN}^B$ gives the upper bound von Neumann entropy for a combined (bipartite) system. Is there a lower bound? For a classical system, the maximum correlation between components A and B would be if, given any state of A then the state of B was fully determined, or vice versa. Although we have not argued this rigorously, it is reasonable that this leads to a minimum entropy equal to the greater of that of system A and B . Hence, the classical (Shannon) entropy obeys $S_{Sh}^{AB} \geq \max(S_{Sh}^A, S_{Sh}^B)$. This corresponds to the very reasonable notion that, for a classical system, the combined system contains at least as much information as any of its components.

In quantum theory, the von Neumann equivalent is the Araki-Lieb inequality, $S_{vN}^{AB} \geq |S_{vN}^A - S_{vN}^B|$. This is difficult to prove, and was first proved only in 1970 [see Araki & Lieb (1970)]. Inequality $S_{vN}^{AB} \geq |S_{vN}^A - S_{vN}^B|$ together with the sub-additivity inequality yield the triangle inequality,

$$|S_{vN}^A - S_{vN}^B| \leq S_{vN}^{AB} \leq S_{vN}^A + S_{vN}^B.$$

Remark. The name derives from the fact that if the entropies of the individual sub-systems are regarded as the lengths of two sides of a triangle, the entropy of the combined system is restricted to the possible lengths of the third side. The Araki-Lieb lower bound entropy is remarkable and displays essentially quantum features. In contrast to the classical case, achieving the Araki-Lieb lower bound entropy implies that the combined system will have less entropy (i.e. less information) than either of its components. Classically this is *incomprehensible*. In quantum mechanics it comes about due to entanglement. For now, consider the entangled state

$\frac{1}{\sqrt{2}}[|\uparrow\rangle_A |\uparrow\rangle_B + |\downarrow\rangle_A |\downarrow\rangle_B]$. Considered as a combined system it is a pure quantum state and hence has zero entropy. But considered as separate sub-systems, each particle can be in one of two states. So the entropy of each sub-system (particle) is 1. The Araki-Lieb inequality is respected because $0 \geq |1-1|$. But notice that each sub-system has greater entropy (1) than the combined system (of zero entropy). There is more information in

each of the parts than in the whole. This non-classical behaviour of quantum information is responsible for the quantum weirdness of entangled states, such as the EPR paradox.

Combined States Strong Subadditivity

In 1973 Lieb and Ruskai proved a stronger inequality, which contains the ordinary subadditivity property as a special case, $S_{vN}^{ABC} + S_{vN}^B \leq S_{vN}^{AB} + S_{vN}^{BC}$.

This may also be written, $S_{vN}^{X \cup Y} + S_{vN}^{X \cap Y} \leq S_{vN}^X + S_{vN}^Y$.

Again it is a major mathematical endeavour to prove this, though simplified derivations have now been presented, e.g. Nielsen & Petz (2005).

Appendix 2

It is well known that the Second Law of thermodynamics is only statistically true. It means that in any process the entropy production is nonnegative on the average, i.e. $\langle \Delta S \rangle \geq 0$, but if wait long enough, then shall see individual events for which the entropy production is negative. This is nicely summarized in the recent fluctuation theorem for the probability of entropy production ΔS as following:

$$\frac{\Pr(\Delta S)}{\Pr(-\Delta S)} = e^{\Delta S}, \text{ or } \Pr(-\Delta S) = \Pr(\Delta S) e^{-\Delta S},$$

implying that negative entropy production events are exponentially rare but not impossible. Negative entropy fluctuations were known much before this modern formulation. In fact, in 1867 Maxwell used the negative entropy fluctuations in a clever thought experiment, involving an imaginary intelligent being — later called Maxwell's Demon — that exploits fluctuations to violate the Second Law. The Demon controls a small frictionless trapdoor on a partition inside a box of gas molecules to sort, without any expenditure of work, faster molecules to one side and slower ones to the other. This gives rise to a temperature gradient from an initially uniform system — a violation of the Second Law. Note that the 'very observant and neat fingered' Demon's 'intelligence' is necessary; a frictionless trapdoor connected to a spring acting as a valve, for example, cannot achieve the same feat.

Maxwell's Demon posed a fundamental challenge. Either such a Demon could not exist, even in principle, or the Second Law itself needed modification. A glimmer of a resolution came with Szilard's reformulation of Maxwell's Demon in terms of measurement and feedback-control of a single-molecule engine. Critically, Szilard emphasized hitherto-neglected information-theoretic aspects of the Demon's operations. Later, through the works of Landauer, Penrose, and Bennett, it was recognized that the Demon's operation necessarily accumulated information and, for a repeating thermodynamic cycle, erasing this information has an entropic cost that ultimately compensates for the total amount of negative entropy production leveraged by the Demon to extract work [12–14]. In other words, with intelligence and information-processing capabilities, the Demon merely shifts the entropy burden temporarily to an information reservoir, such as its memory. The cost is repaid whenever the information reservoir becomes full and needs to be reset. This resolution is concisely summarized in Landauer's principle: the Demon's erasure of one bit of information at temperature T requires at least $k_B T \ln 2$ amount of heat dissipation, where k_B is Boltzmann's constant. (While it does not affect the following directly, it has been known for some time that this principle is only a special case.) Building on this, a modified Second Law was recently proposed that explicitly addresses information processing in a thermodynamic system:

$$\langle \Delta S \rangle + k_B \ln 2 \Delta H \geq 0,$$

where ΔH is the change in the information reservoir's configurational entropy over a thermodynamic cycle information H . These degrees of freedom are coarse-grained states of the reservoir's microstates — the mesoscopic states that store information needed for the Demon's thermodynamic control. Importantly for the following, this Second Law assumes explicitly observed Markov system dynamics and quantifies this relevant information only in terms of the distribution of instantaneous system microstates; not, to emphasize, microstate path entropies. In short, while the system's instantaneous distributions relax and change over time, the information reservoir itself is not allowed to build up and store memory or correlations.

Note that this framework of information reservoirs differs from alternative approaches to the thermodynamics of information processing, including: (i) active feedback control by external means, where the thermodynamic account of the Demon's activities tracks the mutual information between measurement outcomes and system state; (ii) the multipartite framework where, for a set of interacting, stochastic subsystems, the Second Law is expressed via their intrinsic entropy production, correlations among them, and transfer entropy; and (iii) steady-state models that invoke time-scale separation to identify a portion of the overall entropy production as an information current. A unified approach to these perspectives was attempted.

Recently, Maxwellian Demons have been proposed to explore plausible automated mechanisms that appeal to equation (2)'s modified Second Law to do useful work, by decreasing the physical entropy, at the expense of positive change in reservoir Shannon information. Paralleling the modified Second Law's development and the analysis of the alternatives above, they too neglect correlations in the information-bearing components and, in particular, the mechanisms by which those correlations develop over time. In effect, they account for Demon information-processing by replacing the Shannon information of the components as a whole by the sum of the components' individual Shannon information. Since the latter is larger than the former, using it can lead to either stricter or looser bounds than the true bound which is derived from differences in total configurational entropies. More troubling, though, bounds that ignore correlations can simply be violated. Finally, and just as critically, they refer to configurational entropies, not the intrinsic dynamical entropy over system trajectories.

Notably, Demon is highly functional: depending on model parameters, it acts both as an engine, by extracting energy from a single reservoir and converting it into work, and as an information eraser, erasing Shannon information at the cost of the external input of work. Moreover, it supports a new and counterintuitive thermodynamic functionality. In contrast with previously reported erasure operations that only decreased single-bit uncertainty, we find a new kind of erasure functionality during which multiple-bit uncertainties are removed by adding correlation (i.e., by adding temporal order), while single-bit uncertainties are actually increased. This new thermodynamic function provocatively suggests why real-world ratchets support memory: The very functioning of memory full Demons relies on leveraging temporally correlated fluctuations in their environments.

A new Demon proposes for which, for the first time, all correlations among system components can be explicitly accounted. This gives an exact, analytical treatment of the thermodynamically relevant Shannon information change—one that, in addition, accounts for system trajectories not just information in instantaneous state distributions. The result is that, under minimal assumptions, we derive a Second Law that refines by properly accounting for intrinsic information processing reflected in temporal correlations via the overall dynamic's Kolmogorov–Sinai entropy. Conversely, it bounds the thermodynamic cost of any computation. Helpfully, the hidden Markov model (HMM) representations we introduce afford a compact representation of a large class of information reservoirs, much broader than has been considered so far. Moreover, information reservoirs expressed as δ -machines lead to exact analytical treatment.

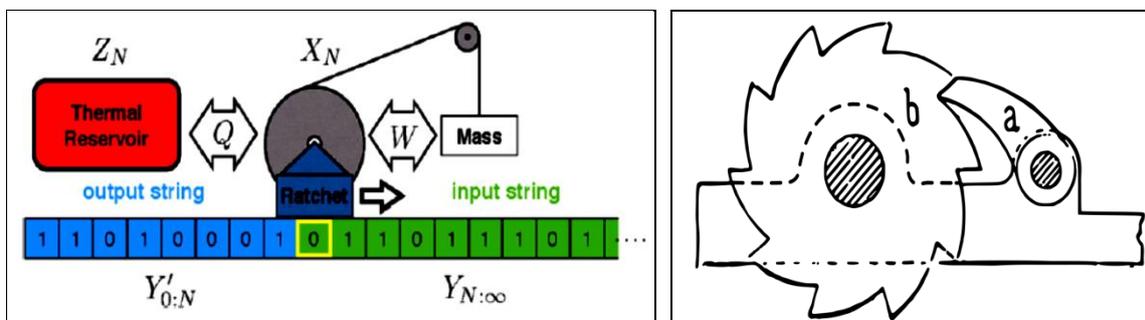


Figure A2.1. Information ratchet sequentially processing a bit string.

Example: Information ratchets Model consists of four components (see Fig. A2.1): 1) an ensemble of bits that acts as an information reservoir; 2) a weight that acts as a reservoir for storing work; 3) a thermal reservoir at temperature T ; and 4) a finite-state ratchet that mediates interactions between the three reservoirs. The bits interact with the ratchet sequentially and, depending on the incoming bit statistics and Demon parameters, the weight is either raised or lowered against gravity. In Fig. 1 at time step N , X_N is the random variable for the

ratchet state and Z_N that for the thermal reservoir. $Y_{N:\infty}$ is the block random variable for the input bit string and $Y'_{0:N}$ that for the output bit string. The last bit Y_N of the input string, highlighted in yellow, interacts with the ratchet. The arrow on the right of the ratchet indicates the direction the ratchet moves along the tape as it sequentially interacts with each input bit in turn.

Remark. As a device that reads and processes a tape of bits, this class of ratchet model has a number of parallels that we mention now, partly to indicate possible future applications. First, one imagines a sophisticated, state full biomolecule that scans a segment of DNA, say as a DNA-polymerase does, leaving behind a modified sequence of nucleotide base-pairs or that acts as an enzyme sequentially catalyzing otherwise unfavorable reactions. Second, there is a rough similarity to a Turing machine sequentially recognizing tape symbols, updating its internal state, and taking an action by modifying the tape cell and moving its read-write head. When the control logic is stochastic, this sometimes is referred to as ‘Brownian computing’. Finally, we are reminded of the deterministic finite-state tape processor that, despite its simplicity, indicates how undecidability can be imminent in dynamical processes. Surely there are other intriguing parallels, but these give a sense of a range of applications in which sequential information processing embedded in a thermodynamic system has relevance.

The bit ensemble is a semi-infinite sequence, broken into incoming and outgoing pieces. The ratchet runs along the sequence, interacting with each bit of the input string step by step. During each interaction at step N , the ratchet state X_N and interacting bit Y_N fluctuate between different internal joint states within $\mathcal{X}_N \otimes \mathcal{Y}_N$, exchanging energy with the thermal reservoir and work reservoir, and potentially changing Y_N 's state. At the end of step N , after input bit Y_N interacts with the ratchet, it becomes the last bit Y'_N of the output string. By interacting with the ensemble of bits, transducing the input string into the output string, the ratchet can convert thermal energy from the heat reservoir into work energy stored in the weight's height. As Fig. 1 illustrates, the state of the overall system is described by the realizations of four random variables: X_N for the ratchet state, $Y_{0:N}$ for the input string, $Y'_{0:N}$ for the output string, and Z_N for the thermal reservoir. A random variable like X_N realizes elements x_N of its physical state space, denoted by alphabet \mathcal{X} , with probability $\Pr(X_N = x_N)$. Random variable blocks are denoted $Y_{a:b} = Y_a Y_{a+1} \dots Y_{b-1}$, with the last index being exclusive. In the following, we take binary alphabets for \mathcal{Y} and \mathcal{Y}' : $y, y' \in \{0, 1\}$. The bit ensemble is considered two joint variables $Y'_{0:N} = Y'_0 Y'_1 \dots Y'_{N-1}$ and $Y_{N:\infty} = Y_N Y_{N+1} \dots$ rather than one $Y_{0:\infty}$, so that the probability of realizing a word $w \in \{0, 1\}^{b-a}$ in the output string is not the same as in the input string. That is, during ratchet operation typically $\Pr Y_{a:b} = w \neq \Pr Y'_{a:b} = w$. The ratchet steadily transduces the input bit sequence, described by the input word distribution $\Pr Y_{0:\infty} \equiv \Pr Y_{0:\infty} = w \quad w \in \{0, 1\}^\infty$ — the probability for every semi-infinite input word — into the output string, described by the word distribution $\Pr Y'_{0:\infty} \equiv \Pr Y'_{0:\infty} = v \quad v \in \{0, 1\}^\infty$. We assume that the word distributions we work with are stationary, meaning that $\Pr Y_{a:a+b} = \Pr Y_{0:b}$ for all non-negative integers a and b .

A key question in working with a sequence such as $Y_{0:\infty}$ is how random it is. One commonly turns to information theory to provide quantitative measures: the more informative a sequence is, the more random it is. For words at a given length ℓ the average amount of information in the $Y_{0:\ell}$ sequence is given by the Shannon block entropy [55]:

$$H Y_{0:\ell} \equiv - \sum_{w \in \{0, 1\}^\ell} \Pr Y_{0:\ell} = w \log_2 \Pr Y_{0:\ell} = w .$$

Due to correlations in typical process sequences, the irreducible randomness per symbol is not the single-symbol entropy $H Y_0$. Rather, it is given by the Shannon entropy rate:

$$h_\mu \equiv \lim_{\ell \rightarrow \infty} \frac{H Y_{0:\ell}}{\ell} .$$

When applied to a physical system described by a suitable symbolic dynamics, as done here, this quantity is the Kolmogorov–Sinai dynamical entropy of the underlying physical behavior.

Note that these ways of monitoring information are quantitatively quite different. For large ℓ , $h_\mu \ell \ll H Y_{0,\ell}$ and, in particular, anticipating later use, $h_\mu \ll H Y_0$, typically much less. Equality between the single-symbol entropy and entropy rate is only achieved when the generating process is memoryless. Calculating the single-symbol entropy is typically quite easy, while calculating h_μ for general processes has been known for quite some time to be difficult and it remains a technical challenge. The entropy rates of the output sequence and input sequence are $h'_\mu = \lim_{\ell \rightarrow \infty} H Y_{0,\ell} / \ell$, respectively. The informational properties of the input and output word distributions set bounds on energy flows in the system. Appendix 2 establishes one of our main results: the average work done by the ratchet is bounded above by the difference in Kolmogorov–Sinai entropy of the input and output processes:

$$\langle W \rangle \leq k_B T \ln 2 (h'_\mu - h_\mu) = k_B T \ln 2 \Delta h_\mu .$$

A complementary interpretation of this new Second Law is that it places a lower bound on the thermodynamic cost (work) to perform information processing and intrinsic computation (change in Shannon entropy of the information reservoir).

In light of the preceding remarks on the basic difference between $H Y_0$ and h_μ , we can now consider more directly the differences between abovementioned equations. Most importantly, the ΔH in the former refers to the instantaneous configurational entropy H before and after a thermodynamic transformation. In the ratchet's steady state operation, ΔH vanishes since the configuration distribution is time invariant, even when the overall system's information production is positive. The entropies h'_μ and h_μ in equation, in contrast, are dynamical: rates of active information generation in the input and output giving, in addition, the correct minimum rates since they take all temporal correlations into account. Together they bound the overall system's information production in steady state away from zero. In short, though often conflated, configurational entropy and dynamical entropy capture two very different kinds of information and they, per force, are associated with different physical properties supporting different kinds of information processing. They are comparable only in special cases.

For example, if one puts aside this basic difference to facilitate comparison and considers the Shannon entropy change ΔH in the joint state space of all bits, the two equations are analogous in the current setup. However, often enough, a weaker version of equation (2) is considered in the discussions on Maxwell's Demon and information reservoirs, wherein the statistical correlations between the bits are neglected, and one simply interprets ΔH to be the change in the marginal Shannon entropies $H Y_0$ of the individual bits. This implies the following relation in the current context:

$$\langle W \rangle \leq k_B \ln 2 \Delta H Y_0 ,$$

where $\Delta H Y_0 = H[Y'_0] - H Y_0$. While this equation is valid for the studies, it can be violated under certain scenarios. In comparison, equation (5) is generally valid. As an example, consider the case where the ratchet has memory and, for simplicity of exposition, is driven by an uncorrelated input process, meaning the input process entropy rate is the same as the single-symbol entropy: $h_\mu = H Y_0$. However, the ratchet's memory can create correlations in the output bit string, so:

$$\Delta h_\mu = h'_\mu - H Y_0 \leq H[Y'_0] - H Y_0 = \Delta H Y_0 .$$

In this case, it is a tighter bound on the work done by the ratchet — a bound that explicitly accounts for correlations within the output bit string generated by the ratchet during its operation. For example, for the ratchet shown in Fig. A2.2 with parameters $\{p = 0.5, q = 0.1\}$ and input bias $\Pr Y_i = 0 = 0.9$, the block

entropies $H[Y'_{0:L}]$ of the output process do not converge to the entropy rate even when looking at block lengths up to $L = 13$.

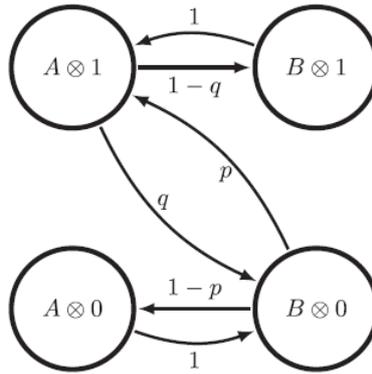


Figure A2.2. The Markovian, detailed-balance dynamic over the joint states of the ratchet and interacting bit.

This means that there are correlations within the output that are not captured even when looking at long blocks of symbols, resulting in an over-estimate of randomness. In short, generally the entropy rate is necessary in order to properly account for the effects of all correlations in the output [55]. Previously, the effect of these correlations has not been calculated, but they have important consequences.

Due to correlations, it is possible to have an increase in the single-symbol entropy difference $\Delta H[Y_0]$ but a decrease in the Kolmogorov–Sinai entropy rate Δh_μ . In this situation, it is erroneous to assume that there is an increase in the information content in the bits. There is, in fact, a decrease in information due to increased correlations. Eq. (5) also has implications for ratchet functioning when the input bits are correlated as well. Specifically, correlations in the input bits can be leveraged by the ratchet to do additional work — work that cannot be accounted for if one only considers single-symbol configurational entropy of the input bits [60].

The availability of heat baths well described by Gibbs states, i.e., states of the form

$$\omega_\beta \triangleq \frac{e^{-\beta H}}{Z_\beta}, \quad Z_\beta \triangleq \text{Tr} e^{-\beta H}$$

with the Hamiltonian H . This description for states in thermal equilibrium can be justified from many different perspectives. The most common ones use some version of a typicality argument, i.e., the statement that most microstates, according to some reasonable measure, give the same measurement statistics for physically relevant observables. Alternatively, one can make use of an ergodic hypothesis together with an argument about the equivalence of ensembles [38]. Quite distinct from these approaches is that of Jaynes' Maximum Entropy Principle. It states that one should always assign that probability distribution (density matrix) to a (quantum) system which is compatible with all the information that one has about its state and otherwise maximizes the Shannon entropy (von Neumann entropy in the quantum case) [31, 32]. Apart from the reasoning based on ergodicity, which, however, seems difficult to translate to the quantum setting since there is no clear notion of ergodicity and non-integrability [63], on the conceptual side these approaches suffer from introducing either some probability measure or an information theoretic entropy measure in an ad-hoc way.

Example. It is in fact not too surprising that it is possible to bring the system to a higher temperature than the heat bath if it was at a colder temperature before. We may imagine that two-level system is a regular thermodynamic system. If it is initially very cold, this means that its non-equilibrium free energy with respect to the environment (exergy) $\Delta F = E - S / \beta - E_\beta - S_\beta / \beta$ is large. Here, E and S denote the initial energy and entropy, respectively, E_β and S_β the corresponding quantities at thermal equilibrium with the environment. We can therefore in principle use a thermodynamic machine to perform an amount of work $W = \Delta F$ while bringing the system into thermal equilibrium. We can then use this amount of work to run a heat-pump and heat up the system above the environment's temperature. It is clear, that by this procedure the free energy

of the system cannot increase, since otherwise we could repeat the procedure and could extract work cyclically from a heat bath. To make connection to the example, let us define the non-equilibrium free energy as

$$\Delta F_{\beta}(\rho, H) \triangleq F_{\beta}(\rho, H) - F_{\beta}(\omega_{\beta}(H), H),$$

with $F_{\beta}(\rho, H) = \text{Tr}(\rho H) - S(\rho) / \beta$ and the von Neumann entropy $S(\rho) = -\text{Tr}(\rho \ln \rho)$. If, for simplicity, we assume that system starts in the ground state and ends in a state with $p' = e^{-\beta \Delta}$ we can then easily see that ΔF_{β} decreases: Since the thermal parts of the free energies cancel, we have (denoting the final state as ρ' and writing $H_S = \Delta|1\rangle\langle 1|$)

$$\begin{aligned} \Delta F_{\beta}(|0\rangle\langle 0|, H_S) - \Delta F_{\beta}(\rho', H_S) &= F_{\beta}(|0\rangle\langle 0|, H_S) - F_{\beta}(\rho', H_S) \\ &= -p' \log p' / \beta - (1-p') \log (1-p') / \beta - p' \Delta = - (1-e^{-\beta \Delta}) \log (1-e^{-\beta \Delta}) / \beta > 0. \end{aligned}$$

This is a general feature of (catalytic) free transitions: The non-equilibrium free energy, defined as ΔF_{β} , can never increase under a (catalytic) free transition. We have seen in this simple example how thermal operations can be used to obtain non-trivial effects, such as population inversions, without having to invest additional "resources". The decisive property of the initial state for this to be possible is that it is far from being in thermal equilibrium with the environment – a property which is in general neither measured by the energy nor the entropy alone. We will return to the general setting and discuss general laws for free transitions akin to the second law of thermodynamics. It was possible to prepare a population inversion from a ground state using free transitions, it was not possible to increase the non-equilibrium free energy ΔF_{β} . This is a general feature of free transitions and show that there are in fact infinitely many functions that can only decrease under (catalytic) free transitions.

Such functions are called *monotones* of the free transitions, since if $\rho \xrightarrow{C} \sigma$, we have $f(\rho) \geq f(\sigma)$ for every monotone f . Hence, they are monotonic with respect to the partial order \xrightarrow{C} induced on states by catalytic free transitions. The importance of monotones comes from the fact that every monotone gives *necessary* conditions for whether a transition $\rho \xrightarrow{C} \sigma$ can be realized as a free transition, i.e., without use of additional non-equilibrium resources. They can therefore be interpreted as second laws of thermodynamics [49]. Using concepts of information theory, it is not difficult find such monotones.

Let us first consider the case of classical information, represented by probability distributions over some set of events X . Suppose we have two such distributions p and q , inferred from some measurement statistics, and want to quantify how different the two distributions are. By applying a (possibly probabilistic) function to X we can obtain new distributions p' and q' on a, possibly different, space of events Y . Such a transformation is called a *post-processing* or *coarse-graining* of the data and clearly it cannot increase the distinguishability between p and q . On the level of the probability distributions, the post-processing is represented by a stochastic matrix T such that $p' = Tp$ and $q' = Tq$. Therefore, an important property of any *measure of distinguishability* D between probability distributions p and q is that it fulfills the *data-processing inequality*: $D(p||q) \geq D(Tp||Tq)$ for every stochastic map T . Similarly, in the case of quantum information, the distinguishability between two quantum states ρ and σ can only decrease under any quantum channel \mathcal{T} . We therefore ask that any sensible measure of distinguishability of quantum states fulfills the corresponding quantum version of the data-processing inequality:

$$D(\rho||\sigma) \geq D(\mathcal{T}(\rho)||\mathcal{T}(\sigma)).$$

We can use this fact to obtain monotones in thermodynamics (or other resource theories) in a quite general fashion. Intuitively, for a system to be out of equilibrium it means that its quantum state is far from being the

Gibbs-state – where the distance is measured with respect to some distinguishability measure between quantum states. Making use of the data-processing inequality, we can now show that this property can only decrease under free transitions:

$$D \rho \|\omega_\beta H \geq D \mathcal{G} \rho \|\mathcal{G} \omega_\beta H = D \mathcal{G} \rho \|\omega_\beta H ,$$

where we have used the fact that free transitions always map Gibbs-states to Gibbs-states.

Any distinguishability measure that fulfills the data-processing inequality automatically defines a monotone of free transitions by setting $f \rho, H = D \rho \|\omega_\beta H$. Important examples of such measures are given by (*quantum*) *Rényi-divergences*. Let us now give the basic definitions that are important for the rest of the thesis, but omit many details. The case that will be most important for us in the following are the (Petz) Rényi divergences defined as

$$D_\alpha \rho \|\sigma = \frac{1}{\alpha-1} \log \text{Tr} \rho^\alpha \sigma^{1-\alpha} .$$

For $0 \leq \alpha \leq 2$, they fulfill the data-processing inequality for arbitrary quantum states when they are well defined.

For general quantum states, we can also define the *minimal quantum Rényi-divergences*

$$\tilde{D}_\alpha \rho \|\sigma = \frac{1}{\alpha-1} \log \text{Tr} \left(\left(\sigma^{\frac{1-\alpha}{2\alpha}} \rho \sigma^{\frac{1-\alpha}{2\alpha}} \right)^\alpha \right) .$$

Both D_α and \tilde{D}_α diverge if the support of ρ is not contained in the support of σ and $\alpha > 1$ and we define them to be equal to $+\infty$ in this case. Similarly, D_α diverges for $\alpha < 0$ if the support of σ is not contained in the support of ρ . While these definitions might at first seem a little bewildering, they have the nice property that

$$\lim_{\alpha \rightarrow 1} D_\alpha \rho \|\sigma = \lim_{\alpha \rightarrow 1} \tilde{D}_\alpha \rho \|\sigma = D \rho \|\sigma ,$$

with the quantum relative entropy D defined as

$$D \rho \|\sigma = \begin{cases} \text{Tr} \rho \log \rho - \text{Tr} \rho \log \sigma & \text{if } \rho \ll \sigma \\ +\infty & \text{otherwise.} \end{cases}$$

Here, $\rho \ll \sigma$ means that the support of the operator ρ is contained in that of σ .

In fact, the quantum relative entropy is nothing but the non-equilibrium free energy in disguise:

$$D \rho \|\omega_\beta H = \beta \Delta F_\beta \rho, H ,$$

as can be checked by a simple direct calculation. All the quantum Rényi-divergences are additive over tensor-products and hence also provide monotones of catalytic free transitions. We thus arrive at the important insight that the non-equilibrium free energy ΔF_β , and its cousins defined using (quantum) Rényi-divergences for different values of α , are monotones of catalytic free transitions. They can never increase in a free transitions.

In many applications, we can make the simplifying assumption that all states in question commute with the Hamiltonian, i.e., are time-invariant. In this case, drastic simplifications occur.

First, the minimal quantum Rényi-divergences simplify to the classical Rényi-divergences:

$$D_\alpha \rho \parallel \sigma = \tilde{D}_\alpha \rho \parallel \sigma ,$$

if $\rho, \sigma = 0$.

Second, we have the following important result, which shows that the Rényi-divergences not only imply necessary conditions for a catalytic free transition, but also provide sufficient conditions.

Example: Stochastic thermodynamics and fluctuation relations The concept of fluctuation relations had big impact on the field of statistical mechanics. It originates from studying stochastic thermodynamics, which is concerned with the thermodynamic properties of individual particles which can come in contact with heat baths. In stochastic thermodynamics, the particle in question undergoes dynamical trajectories under influence of stochastic forces, leading to stochastic notions of basic properties in thermodynamics, such as entropy production, heat dissipation or work being done by or on the particle. Fluctuation relations provide, under quite general assumptions, detailed and universal relations for the probability distributions of various quantities, such as the work being done by the particle along a trajectory.

“INFORMATION IS PHYSICAL” in the sense that it has to be represented by states of physical systems. Landauer argued that this implies that the erasure of information then in general leads to irreversible dissipation of heat by an amount $k_B T \log 2$, where T is the environment temperature. We will now explain how this bound follows from the previous considerations about monotones. This is of course not a new result, but serves as a simple illustration of the framework. We imagine a physical two-level systems (with Hamiltonian H_S), whose levels encode a single bit of information. To erase the information encoded in the system means to reset its state to $|0\rangle$ (or any other fixed, pure reference state), independent of the initial state. We want to achieve this using a (catalytic) free transition. On the one hand, using such a thermal operation, we can always thermalize the system to the environment’s temperature for free, for example by swapping first the system with an identical, but thermalized two-level system from the environment. On the other hand, the bit erasure also has to work if the system is initially already thermalized. We will therefore consider without loss of generality the situation in which the initial state of the system is a thermal state.

The first observation that we make is that since the system is initially in equilibrium with the bath, a thermal operation without any additional system cannot be used to erase the bit, because thermal operations cannot bring a system out of equilibrium. We thus have to have access to an additional system, which we call "resource", with a quantum state ρ_R and Hamiltonian H_R . We assume that this resource is initially uncorrelated with the bit. Let the final state of the resource be ρ'_R . From the monotonicity and additivity of the free energy we then get:

$$\begin{aligned} \Delta F_\beta \rho_R \otimes \omega_\beta H_S, H_R + H_S &= \Delta F_\beta \rho_R, H_R \geq \Delta F_\beta \rho'_R \otimes |0\rangle\langle 0|, H_R + H_S \\ &= \Delta F_\beta \rho'_R, H_R + \Delta F_\beta |0\rangle\langle 0|, H_S , \end{aligned}$$

where we have used that a system in a pure state cannot be correlated to another system.

Since $\Delta F_\beta |0\rangle\langle 0|, H_S = 0 - E_\beta + S_\beta / \beta$ we thus obtain:

$$F_\beta \rho_R, H_R - F_\beta \rho'_R, H_R \geq k_B T S_\beta - E_\beta.$$

Here, S_β and E_β denote the thermal entropy and energy of the bit to be erased. Let us consider some special cases:

1	If the Hamiltonian of the bit does not discriminate between the two level $H_S \propto 1$, we obtain $F_{\beta}(\rho_R, H_R) - F_{\beta}(\rho'_R, H_R) \geq k_B T \log 2$
2	In the case where the state of the resource system does not change its entropy, we may want to interpret the change of energy on it as "work" provided by the resource (see, however, chapter 4). In this case we get $W \geq k_B T \log(2)$.
3	In the case where the resource system does not change its energy, but only its entropy, we see that its entropy has to increase at least by the thermal entropy of the bit S_{β} . We can then say that an amount of heat $Q = TS_{\beta}$ has been generated in the resource.

Intuitively, it should be easier to erase the information, if we have some knowledge about the state of the bit before we want to erase it. For example, if the bit is known to be in state $|1\rangle$ and H_S is trivial, then we can simply flip the spin and no resource is necessary. Let us now demonstrate in general how such correlations affect the erasure bound in a simple example.

Example. Since information is physical, having prior knowledge means that there exists a physical system which is correlated with the bit. We will call this system a memory M . The memory and system together are initially in some correlated state described by the density matrix ρ_{SM} . To simplify the problem, let us assume $H_S \propto 1$ and $H_M \propto 1$, and assume that the initial state on S is maximally mixed, $\rho_S = 1/2$. The final state of the system definitely is $|0\rangle$ and is hence uncorrelated with the memory. We will now make the restriction that the memory ends up in the same internal state ρ_M since we want to highlight only the effect of the correlations. In principle, if ρ_M is not given by the maximally mixed state, we could tasks. Summarizing, we thus find that the initial entropy of SM is given by $S(\rho_{SM})$ and the final entropy by $S(\rho_M)$. Arguing as above by regarding the compound SM as a single system, we then find

$$F_{\beta}(\rho_R, H_R) - F_{\beta}(\rho'_R, H_R) \geq k_B T (S(\rho_{SM}) - S(\rho_M)) = k_B T H(S|M)_{\rho'}$$

where we have introduced the *conditional entropy* $H(S|M)_{\rho} = S(\rho_{SM}) - S(\rho_M)$, which is a measure for the information about S contained in M . Interestingly, in quantum mechanics, the conditional entropy can be negative if the initial state ρ_{SM} is entangled. In such a case, one can in principle *extract non-equilibriumness* by erasure instead of investing nonequilibriumness to erase information.

We have seen how the formalism of thermal operations allows us to derive in a simple way the fundamental Landauer bound including side-information. However, we have only derived necessary conditions for erasure. In particular, we did not make use of theorem, which tells us that we should check the infinite family of second laws given by the Rényi divergences. We will come back to this problem below, where we will find that there are much more stringent conditions than just Landauer's bound when we want to bring a system to the ground state, which can be interpreted as a quantitative version of the third law of thermodynamics.

In the context of quantum mechanics, a simple fluctuation relation is concerned with the energy fluctuations when a system that is initially in thermal equilibrium undergoes unitary dynamics. To understand the relation, consider the following operational protocol. Assume we have a system initially in a thermal state. First we perform an energy measurement, obtaining an outcome E^i and projecting the state of the system to the energy eigenstate $|E^i\rangle$. Then we let the system undergo unitary dynamics \mathcal{U} , which possibly changes the Hamiltonian over time and is not required to conserve the energy. Then we measure again the final energy to obtain some outcome E^f . Repeat the experiment many times and determine the distribution $P(\Delta E)$ of the random variable $\Delta E = E^i - E^f$. Then the distribution $P(\Delta E)$ fulfills the *Jarzynski equation*

$$\mathbb{E} e^{\beta \Delta E} = \frac{Z_{\beta} H^f}{Z_{\beta} H^i},$$

where $\mathbb{E} \bullet$ denotes the expectation value of a random variable. Often, the energy-difference ΔE is interpreted as fluctuating, mechanical work being done by the system. Indeed, using Jensen's inequality, we can obtain the inequality $\mathbb{E} \Delta E \leq F_{\beta} H^i - F_{\beta} H^f$, which can then be interpreted as an expression of the second law of thermodynamics relating work to free energy changes. On the other hand, it is an *equality* which contains information about higher cumulants of ΔE and hence provides more detailed information about possible fluctuations of work. Fluctuation relations can, however, also be de-rived under different assumptions in the quantum regime and there is by now a vast body of literature dealing with fluctuation relations in the quantum setting. It is then probably not surprising that similar relations can also be derived in the framework of thermal operations.

Example. To derive such relations in the framework of thermal operations, it is necessary to introduce an auxiliary system W which can take up energy from the system of interest or give energy to it. Here, we will take the stance that this external energy is supposed to model intuitively what one considers to be mechanical work. Such a system should then have the property that it resembles the classical notion of "lifted weight", being able to take up and release arbitrary amounts of energy. Furthermore, the weight should not act as an entropy sink. Finally, at least the average work provided by the weight or done on the weight should not be dependent on the initial state of the weight. The classical Jarzynski relation can then be recovered if one additionally assumes that the induced map on the system and *weight* Γ_{SW} maps energy eigenstates to mixtures of energy-eigenstates. We will now present a formal derivation of this result. In this classical case, the action on SW for states diagonal in the energy-eigenbasis can be represented by conditional probabilities $P_{E_{S'}, w}$:

$$\Gamma_{SW} |E_S\rangle\langle E_S| \otimes |0\rangle\langle 0| = \sum_{S', w} P_{E_{S'}, w} |E_{S'}\rangle\langle E_{S'}| \otimes |x+w\rangle\langle x+w|,$$

where $|x\rangle$ denote (generalized) energy-eigenstates of the weight and E_S is the spectrum of H_S . Due to the commutation constraint $\mathcal{U}, P = 0$, the conditional probabilities $P_{E_{S'}, w} |E_S$ are in fact independent of the initial state on the weight as long as the initial state on W is diagonal in the position basis (this excludes the possibility of a purely unitary dynamics on the system and bath and is analogous to the requirement of performing energy-measurements before and after a protocol in different frameworks). One can thus choose without loss of generality that this state is $|0\rangle$ and refer to the event that this state is changed to a state $|w\rangle$ as extracting an *amount of work* w . The quantity $P_{E_{S'}, w} |E_S$ then denotes the conditional probability that the system goes from an energy eigenstate $|E_S\rangle$ to an energy eigenstate $|E_{S'}\rangle$ while an amount of work w is extracted.

In the field of open system dynamics, a seminal observation was that one can in this case define an entropy production function as: $\sigma_t = -\frac{d}{dt} D(\rho_t) \|\omega_{\beta} H$, which is always non-negative due to the data-processing inequality: $\sigma_t \geq 0$. It is natural to interpret this inequality as an expression of the second law of thermodynamics.

4. Appendix 3

The second law of thermodynamics places constraints on state transformations. It applies to systems composed of many particles. However, we are seeing that one can formulate laws of thermodynamics when only a small number of particles are interacting with a heat bath. The second law for microscopic systems takes on a different form compared to the macroscopic scale, imposing not just one constraint on state transformations,

but an entire family of constraints. It was find a family of free energies which generalize the traditional one, and show that they can never increase. The ordinary second law relates to one of these, with the remainder imposing additional constraints on thermodynamic transitions. It was find three regimes which determine which family of second laws governs state transitions, depending on how cyclic the process is. In one regime one can cause an apparent violation of the usual second law, through a process of embezzling work from a large system which remains arbitrarily close to its original state. These second laws are relevant for small systems, and also apply to individual macroscopic systems interacting via long-range interactions.

By making precise the definition of thermal operations, the laws of thermodynamics are unified in this framework, with the first law defining the class of operations, the zeroth law emerging as an equivalence relation between thermal states, and the remaining laws being monotonicity of generalized free energies. At the macroscopic scale, and for systems with short-range correlations, this entire family of second laws becomes equal to the ordinary second law, but outside of this regime these other second laws impose additional restrictions on thermodynamical transitions. What is more, one needs to be more precise about what one means by a cyclic process. At the macroscopic scale, the fact that a process is only approximately cyclic has generally been assumed to be enough to guarantee the second law. This is not the case in the microscopic regime, and therefore needs to talk about “how cyclic” a process is when stating the second law. For thermodynamics at the macroscopic scale, a system in state ρ can be transformed into state ρ' provided that the free energy goes down, where the free energy for a state ρ is $F(\rho) = \langle E(\rho) \rangle - kTS(\rho)$, with T the temperature of the ambient heat bath that surrounds the system, k the Boltzmann constant, $S(\rho)$ the entropy of the system, and $\langle E \rangle$ its average energy. It tells us whether a system at constant volume and in contact with a heat bath can make a spontaneous thermodynamical transition from one state to another. A transition can only happen if the free energy of the final state is lower than that of the initial state. The difference in free energy between the initial and final state is also the amount of work that can be extracted from a system in a thermal bath. It also gives the amount of work required to perform the reverse process, as thermodynamics at the macroscopic scale is reversible.

This is a version of the second law, where also the fact that the total energy of the system and heat bath must be conserved is used. This criterion governing state transitions is valid if the system is composed of many particles, and there are no long-range correlations. In the case of microscopic, quantum, or highly correlated systems, a criterion for state transitions of a total system was proven and named thermo-majorization. This criterion has been conjectured and serves as a second law in some cases. However, here we will see that if elevated to such high status without sufficient care, it can be violated. Namely, we will give examples where $\rho \rightarrow \rho'$ would violate the thermo-majorization criterion, but nonetheless, the transition is possible via a cyclic process in which a working body σ — an ancilla or catalyst — is returned back into its original state. The criterion is thus only relevant when additional systems are not used to aid in the transition. Instead of considering macroscopic work (the pushing out of a piston or the raising of a weight), consider microscopic work — for example, the exciting of an atom from its ground state to an excited state (Fig. A3.1). However, as above-mentioned, the free energy is only valid in the thermodynamical limit—when ρ is composed of many particles and is classical, in the sense that it is in a state that is a probabilistic mixture of different energies. However, thermodynamical effects are not only important in the macroscopic regime — they are becoming increasingly important as we probe and manipulate small systems from the micro up to the mesoscopic scale.

Remark. Having many of these atoms would allow us to perform macroscopic work — for example, we could use the atoms in a laser. An amount of work W can be used to produce a transition from the state $|0\rangle\langle 0|$ to the state $|1\rangle\langle 1|$, with Hamiltonian $\hat{W} = W|1\rangle\langle 1|$ (we call such a two-level system the work qubit or wit). We can use such a system as a basic work storage unit, as our results will not depend on what physical system is used. We can thus use a two-level system to store work. As the amount of extractable work can be small, we require precise accounting of all sources of energy. We thus consider a paradigm where extraction of work, and other operations, must be done using energy-conserving operations, so that any energy that is transferred to or from the resource system and heat bath is transferred from or to the system that stores work. We thus consider a paradigm where extraction of work, and other operations, must be done using energy-conserving operations, so that any energy that is transferred to or from the resource system and heat bath is transferred from or to the system that stores work. We do not impose any additional constraints, as we wish to explore fundamental limitations on what can be accomplished on work extraction and formation.

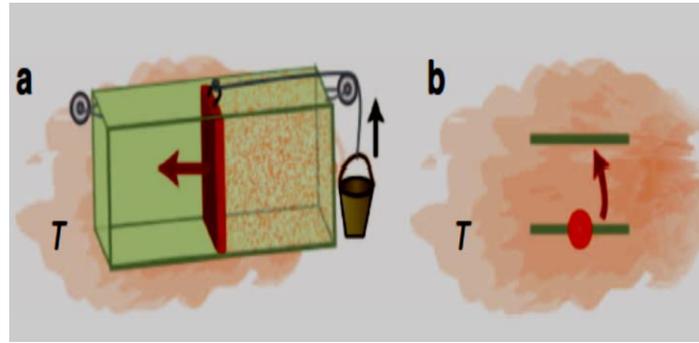


Figure A3.1. Macroscopic and microscopic work. (a) A macroscopic heat engine that performs work by lifting a heavy weight a certain height. (b) In the quantum or micro-regime, we can think of work as the ability to excite a two-level system from one energy state to a higher one.

We call the class of operations that are allowed Thermal Operations including how it is related to other natural paradigms.

Definition of Thermal Operations. We will first consider a quantum system $\rho = \sum \sigma_{E, E', g, g'} |E, g\rangle\langle E, g|$ with a fixed Hamiltonian H and eigenstates of energy E given by $|E, g\rangle$, in contact with a heat bath. We are interested in the types of state transitions that are allowed and, in particular, our ability to use the system as a resource to extract work. We will then consider the case where the Hamiltonian of the initial and final state is not the same, so that the system undergoes a non-cyclic evolution.

This casts thermodynamics as a *resource* theory, which allows us to exploit some mathematical machinery from information theory. Thermodynamics is then viewed as a theory involving state transformations in the presence of a thermal bath. The extraction or expenditure of work can be included in such a paradigm, because it is equivalent to a state transformation — the state of the work qubit is raised or lowered from one energy eigenstate to another.

Extractable work. In the macroscopic regime, and for systems which are not highly correlated, then $F_\alpha(\rho, \rho_\beta) \approx F_1(\rho, \rho_\beta)$ for all α , which explains why the single constraint given by the usual second law is more or less adequate in this limit. It was previously found that the quantity $F_{\min}(\rho)$, defined as $F_{\min}(\rho) = -kT \ln \sum h(\omega, g, E_i) e^{-\beta E_i}$, where $\omega = \sum_E P_E \rho_E P_E$ with $P_E = |E\rangle\langle E|$ is the state ρ decohered in the energy eigenbasis (that is, off-diagonal terms are set to zero), $h(\omega, g, E_i)$ is 1 if energy level $|g, E_i\rangle$ is populated and 0 otherwise, β is the inverse temperature, and k is Boltzmann's constant, gives the maximal amount of work extractable from a system in contact with a reservoir under all thermal operations (by transforming it to a thermal state in equilibrium with the bath). This is also the relevant quantity in a model of alternating adiabatic and isothermal operations. In terms of information-theoretic quantities, we can write as $F_{\min}(\rho) - F_{\min}(\theta) = kTD_{\min}(\rho \parallel \theta)$, where $D_{\min}(\rho \parallel \theta) = -\ln \text{Tr} \Pi_\omega \theta$ is the *min-relative entropy* with Π_ω the projector onto the support of ω and θ is the Gibbs state $\theta = Z^{-1} \sum_{E, g} e^{-\beta E} |E, g\rangle\langle E, g|$ with partition function Z . The min-relative entropy and single-shot free energy has been independently introduced as a lower bound for work extraction from classical states using a model of a series of independent interactions with a heat bath. In the thermodynamical limit $D_{\min}(\rho \parallel \theta)$ becomes the relative entropy $S(\rho \parallel \theta) = -\text{Tr} \rho \log \theta + \text{Tr} \rho \log \rho$, which is equal to $F(\rho) - F(\theta)$. Thus, while the maximum amount of work W that can be extracted when a macroscopic system is in contact with a heat bath is $W = F(\rho) - F(\theta)$, more generally it is $W = F_\epsilon^{\min}(\rho) - F_\epsilon^{\min}(\theta)$, where a β -smoothed version of F_{\min} , called F_ϵ^{\min} , gives the optimal and achievable amount of work extractable from the resource and only in the thermodynamical limit do we recover the traditional result. The finite size of the system means that less work can be extracted. There

is a second reason why a limitation exists on the amount of extractable work. As an example, consider the pure

$$\text{quantum state } |\psi\rangle = \sum_E \sqrt{\frac{e^{-\beta E}}{Z}} |E\rangle.$$

It has entropy and rank equal to zero. However, when dephased in the energy eigenbasis to produce ω , it becomes the Gibbs state if the energy levels are non-degenerate, and has free energy $-kT \ln Z$, no work can be extracted from it, despite it having zero entropy. However, as we approach the thermodynamic limit, the coherences matter less and less, and the free energy in the quantum case approaches the free energy for classical states and, again, F_{\min} approaches the Helmholtz free energy.

Remark. In general, $F_{\varepsilon}^{\min} \rho \leq F \leq F_{\varepsilon}^{\max} \theta$, so that at the nanoscale we can generally extract less work from a resource than is required to create the resource, leading to a fundamental irreversibility in thermodynamical processes. In terms of information-theoretic quantities, $F_{\max} \rho - F_{\max} \theta = TD_{\max} \rho \parallel \theta$, where $D_{\max} \rho \parallel \theta = \log \min \lambda : \rho \leq \lambda \theta$ is the max-relative entropy. As we approach the thermodynamic limit $F_{\varepsilon}^{\min} \rho \approx F_{\varepsilon}^{\max} \theta$, reversibility is restored.

Example: Changing Hamiltonians We introduce a qubit on system C that we can act on to switch the Hamiltonian from H to H' (we call this the switching qubit). We can, for example, take the total Hamiltonian to be $H_{tot} = |0\rangle\langle 0|_C \otimes H + |1\rangle\langle 1|_C \otimes H' + W|1\rangle\langle 1|$ and take the initial state of the work qubit, switching qubit and system to be $|00\rangle\langle 00|_{CW} \otimes \rho$ and final state to be $|11\rangle\langle 11|$, so that we are effectively changing the Hamiltonian acting on ρ , and gaining or losing work in the work qubit when we make the transition to σ . We now consider a transition between ρ and θ' , the thermal state with Hamiltonian H' , and want to know what value (positive or negative) for W allows us to make this transition. The results, obtained by means of thermomajorization, are one finds $W = F_{\varepsilon}^{\min} \omega - F_{\varepsilon}^{\min} \theta'$ for extracting work, and for the amount of work required to form ρ (provided it is diagonal in energy eigenbasis) from the thermal state, we obtain $W = F_{\varepsilon}^{\max} \omega - F_{\varepsilon}^{\max} \theta'$. This result does not depend on the form of the Hamiltonian of H_{tot} — only require that at late times, there is no interaction between the work qubit and the systems (as we need to be able to separate out the work qubit to use in some future process). More general state-to-state transformations assisted by work are also depicted.

Remark. The case where we adjust W so that $\rho \otimes |00\rangle\langle 00|_{CW}$ is thermomajorized by $\sigma \otimes |11\rangle\langle 11|_{CW}$ gives us the work required / distillable for a general transformation, while setting $\rho = \theta$ gives the formation process and free energy of $W = F_{\varepsilon}^{\max} \omega - F_{\varepsilon}^{\max} \theta'$. The case where both initial and final states ρ and σ are thermal leads to the ideal classical result, namely that a transition is possible if and only if $W = -kT \ln Z / Z'$ that is, the work is given by the difference of standard free energies $F \rho = \langle E \rho \rangle - kTS \rho$.

In 1961, Alfred Rényi defined a parametrized family of entropies now bearing his name, by relaxing one of the axioms that singles out the Shannon entropy. This led to both the α – Rényi entropy and the α – Rényi divergence, defined respectively for a parameter $\alpha \in 0, 1 \cup 1, \infty$ and probability distributions p and q as

$$H_{\alpha} p = \frac{1}{1-\alpha} \log \sum_x [p(x)]^{\alpha}, \quad D_{\alpha} p \parallel q = \frac{1}{1-\alpha} \log \sum_x [p(x)]^{\alpha} [q(x)]^{1-\alpha}.$$

The Shannon entropy and relative entropy are recovered in the limit as $\alpha \rightarrow 1$:

$$\lim_{\alpha \rightarrow 1} H_{\alpha} p = H p \equiv -\sum_x p(x) \log p(x), \quad \lim_{\alpha \rightarrow 1} D_{\alpha} p \parallel q = D p \parallel q \equiv -\sum_x p(x) \log \frac{p(x)}{q(x)}.$$

Part of what makes the Rényi entropies so useful in applications is their properties: convergence to the Shannon and relative entropies in the limit as $\alpha \rightarrow 1$, monotonicity in the parameter α , and additivity, in addition to others. The convergence to the Shannon and relative entropies ensures that, by taking this limit, one recovers asymptotic information-theoretic statements, such as the data compression theorem or the channel capacity theorem, from the more fine-grained statements. Monotonicity in the parameter α ensures that $H_\alpha p$ gives more weight to low surprisal events for $\alpha > 1$ and vice versa for $\alpha < 1$, helping to characterize the aforementioned trade-off in informationtheoretic settings. The additivity property implies that the Rényi entropies can simplify immensely when evaluated for memoryless stochastic processes. With the intent of developing either a multipartite classical or quantum generalization of (1.1), one might suggest after a moment’s thought to replace a quantity which features a linear combination of entropies by one with the same linear combination of Rényi entropies. However, this approach is objectively unsatisfactory in at least two regards: properties of the original information measure are not preserved by doing so and one is not guaranteed to have the powerful monotonicity in α property mentioned above. For example, take the case of the conditional mutual information of a tripartite density operator ρ_{ABC} defined as

$$I(A;B|C)_\rho = H(AC)_\rho + H(BC)_\rho - H(C)_\rho - H(ABC)_\rho,$$

where $H(F)_\rho \equiv -\text{Tr}(\sigma_F \log \sigma_F)$ is the quantum entropy of a density operator σ on system F .

One of the most important properties of this quantity is that it is non-negative (known as strong

subadditivity of quantum entropy), and as a consequence, it is monotone nonincreasing with respect to any quantum channel applied to the system A (by symmetry, the same is true for one applied to B). However, if we define a Rényi generalization of $I(A;B|C)_\rho$ as $H_\alpha(AC)_\rho + H_\alpha(BC)_\rho - H_\alpha(C)_\rho - H_\alpha(ABC)_\rho$,

where $H_\alpha(F)_\sigma \equiv \left[\log \text{Tr}(\sigma_F^\alpha) \right] / (1-\alpha)$, then explicit counterexamples reveal that this Rényi generalization can be *negative*, monotonicity with respect to quantum channels need not hold, and neither does monotonicity in α .

Remark. Continuing with the abovementioned example of conditional mutual information, consider the following Rényi generalization

$$I_\alpha(A;B|C)_\rho \equiv \frac{1}{\alpha-1} \log \text{Tr}(\rho_{ABC}^\alpha \rho_{AC}^{1-\alpha/2} \rho_C^{1-\alpha/2} \rho_{BC}^{1-\alpha/2} \rho_C^{1-\alpha/2} \rho_{AC}^{1-\alpha/2}).$$

For $\alpha \in (0,1) \cup (1,2)$, the quantity is non-negative, monotone non-increasing with respect to quantum channels acting on the B system, converges to $I(A;B|C)_\rho$ in the limit as $\alpha \rightarrow 1$, and is conjectured to obey the monotonicity in α property (with some numerical and analytical evidence in favor established). However, hitherto a proof of the monotonicity in α property for

$I_\alpha(A;B|C)_\rho$ remains lacking. It is also an open question to determine whether $I_\alpha(A;B|C)_\rho$ is monotone non-increasing with respect to quantum channels acting on the A system — this partially has to do with the fact that $I_\alpha(A;B|C)_\rho$ is not symmetric with respect to exchange of the A and B systems, unlike the conditional mutual information.

Generalized measures of entropies and information The modification of the recently proposed Rényi generalizations of quantum information measures by placing “swivels” in a given chain of operators. As an example of the idea, consider that we can rewrite the quantity $I_\alpha(A;B|C)_\rho$ in terms of the Schatten 2-norm as follows:

$$I'_\alpha(A;B)_\rho \equiv \frac{2}{\alpha-1} \max_{V_A \in \mathbb{V}_{\rho_A}} \log \left\| \rho_B^{1-\alpha/2} \rho_A^{1-\alpha/2} V_{\rho_A} \rho_{AB}^{\alpha/2} \right\|_2.$$

The new idea is to modify this quantity to include swivels as follows:

$$I'_{\alpha} A;B_{\rho} \equiv \frac{2}{\alpha-1} \max_{V_{\rho_{AC}} \in \mathbb{V}_{\rho_{AC}}, V_{\rho_C} \in \mathbb{V}_{\rho_C}} \log \left\| \rho_{BC}^{1-\alpha/2} V_{\rho_C} \rho_C^{1-\alpha/2} \rho_{AC}^{1-\alpha/2} V_{\rho_{AC}} \rho_{ABC}^{\alpha/2} \right\|_2.$$

where \mathbb{V}_{ω} is the compact set of all unitaries V_{ω} commuting with the Hermitian operator ω . Thus, the fixed eigenbases of ρ_C and ρ_{AC} act as swivels connecting adjacent operators in the operator chain above, such that the unitary rotations V_{ρ_C} and $V_{\rho_{AC}}$ about these swivels are allowed. Such swivels make no difference when the density operator ρ_{ABC} and its marginals commute with each other (the classical case), or when the C system is trivial, in which case the above quantity reduces to a Rényi mutual information

$$I'_{\alpha} A;B_{\rho} \equiv \frac{2}{\alpha-1} \max_{V_{\rho_A} \in \mathbb{V}_{\rho_A}} \log \left\| \rho_B^{1-\alpha/2} \rho_A^{1-\alpha/2} V_{\rho_A} \rho_{AB}^{\alpha/2} \right\|_2 = \frac{2}{\alpha-1} \log \left\| \rho_B^{1-\alpha/2} \rho_A^{1-\alpha/2} \rho_{AB}^{\alpha/2} \right\|_2.$$

The swiveled Rényi entropies are in general discontinuous at $\alpha = 1$ and do not converge to the von Neumann entropy-based measures in the limit as $\alpha \rightarrow 1$.

Family of Second Laws Here, we consider all possible cyclic thermodynamical processes, and show that transition laws are affected by using ancillary systems which are returned back to their initial state. Rather than a single free energy that determines which transitions are possible, we find necessary and sufficient conditions for thermodynamic transitions which form not just one but a family of second laws. We define the free energies

$$F_{\alpha} \rho, \rho_{\beta} = kTD_{\alpha} \rho \left\| \rho_{\beta} \right. - k \log Z, \quad \text{with the Rényi divergences } D_{\alpha} \rho \left\| \rho_{\beta} \text{ defined as}$$

$$D_{\alpha} \rho \left\| \rho_{\beta} = \frac{\text{sgn } \alpha}{\alpha-1} \log \sum_i p_i^{\alpha} q_i^{1-\alpha}, \quad \text{where } p_i \text{ are the eigenvalues of } \rho \text{ and } q_i \text{ the eigenvalues of the thermal state of the system } \rho_{\beta} = e^{-\beta H_S} / Z \text{ with Hamiltonian } H_S, \text{ partition function } Z = \sum_i e^{-\beta E_i}, \text{ and } \beta = 1/T.$$

We can then state quantum second laws, and ones that hold for states block diagonal in the energy basis. In the latter case, we find the following set of second laws: In the presence of a heat bath of single fixed temperature, the free energies $F_{\alpha} \rho, \rho_{\beta}$ do not increase for $\alpha \geq 0$. That is, $\forall \alpha \geq 0, F_{\alpha} \rho, \rho_{\beta} \geq F_{\alpha} \rho', \rho_{\beta}$, where ρ and ρ' are the initial and final state, respectively. Moreover, if $F_{\alpha} \rho, \rho_{\beta} \geq F_{\alpha} \rho', \rho_{\beta}$ holds $\forall \alpha \geq 0$, then there exists a catalytic thermal operation that transforms ρ to ρ' . For $\alpha \rightarrow 1$, $F_{\alpha} \rho, \rho_{\beta}$ is equal to the ordinary Helmholtz free energy $F \rho$, hence the conditions include the ordinary second law (combined with energy conservation), and we thus see that it is merely one of many constraints on thermodynamical state transitions.

We see this in newly derived second laws as well, for at $\alpha = 0, F_0 \rho, \rho_{\beta} = F_{\min} \rho$.

For states that are not diagonal in the energy basis, a generalization of the above limitations in terms of quantum alpha-free energies was we provided. These form a family of fully quantum second laws, which are necessary but not sufficient conditions for state transformations. Due to the noncommutative nature of the state of the system and the thermal state, our new free energies have a more complicated form and are based on quantum Rényi divergences. Defining two quantum versions of $F_{\alpha} \rho, \rho_{\beta}$ as following:

$$\tilde{F}_{\alpha} \rho, \rho_{\beta} = kT \frac{\text{sgn } \alpha}{\alpha-1} \log \text{Tr} \rho^{\alpha} \rho_{\beta}^{1-\alpha} - kT \log Z$$

and

$$\hat{F}_\alpha \rho, \rho_\beta = kT \frac{1}{\alpha-1} \log \text{Tr} \rho_\beta^{1-\alpha/2\alpha} \rho \rho_\beta^{1-\alpha/2\alpha} - kT \log Z,$$

it is able to find

Quantum second laws

A transition from ρ to ρ' is possible, only if

$$\hat{F}_\alpha \rho, \rho_\beta \geq \hat{F}_\alpha \rho', \rho_\beta \quad \text{for } \alpha \geq \frac{1}{2} \text{ and}$$

$$\hat{F}_\alpha \rho_\beta, \rho \geq \hat{F}_\alpha \rho_\beta, \rho' \quad \text{for } \frac{1}{2} \leq \alpha \leq 1 \text{ and}$$

$$\tilde{F}_\alpha \rho, \rho_\beta \geq \tilde{F}_\alpha \rho', \rho_\beta \quad \text{for } 0 \leq \alpha \leq 2,$$

where once again the above laws include transitions where the Hamiltonian changes by making use of an ancillary system.

Remark: Generalized measures of quantum Rényi divergences We shall recall the definition of the $\alpha - z$ relative Rényi entropies:

$$D_{\alpha,z} \rho \parallel \sigma = \frac{1}{\alpha-1} \log \text{Tr} \left(\left(\sigma^{\frac{1-\alpha}{2z}} \rho^z \sigma^{\frac{1-\alpha}{2z}} \right)^z \right), \quad \alpha \in \mathbb{R} \setminus 1, z \in \mathbb{R} \setminus 0.$$

We will refer the $\alpha - z$ relative Rényi entropies as $\alpha - z$ divergences for convenience. Indeed, we have

$$D_{\alpha,1} \rho \parallel \sigma = D_\alpha \rho \parallel \sigma = \frac{1}{\alpha-1} \log \text{Tr} \sigma^{1-\alpha} \rho^\alpha,$$

$$D_{\alpha,\alpha} \rho \parallel \sigma = \tilde{D}_\alpha \rho \parallel \sigma = \frac{1}{\alpha-1} \log \text{Tr} \left(\left(\sigma^{\frac{1-\alpha}{2\alpha}} \rho \sigma^{\frac{1-\alpha}{2\alpha}} \right)^\alpha \right).$$

For the case $\sigma \gg \rho$ $D_{\alpha,1} \rho \parallel \sigma$ and $D_{\alpha,\alpha} \rho \parallel \sigma$ are differentiable at $\alpha = 1$, and we have

$$\left. \frac{d}{d\alpha} D_{\alpha,1} \rho \parallel \sigma \right|_{\alpha=1} = \left. \frac{d}{d\alpha} D_{\alpha,\alpha} \rho \parallel \sigma \right|_{\alpha=1} = \frac{1}{2} V \rho \parallel \sigma,$$

where $V \rho \parallel \sigma \triangleq \text{Tr} \rho \log \rho - \log \sigma^2 - \text{Tr} \rho \log \rho - \log \sigma^2$ is the relative entropy variance.

Derivation of the second laws is information theoretic in nature, requiring none of the assumptions usually required for the second law to hold. This includes ergodicity, mixing, coarsegraining of degrees of freedom, and lack of control over the system. Monotonicity of $F_\alpha \rho, \rho_\beta$ thus provides a powerful tool to determine what sorts of thermodynamical transitions are possible on the quantum scale, or equally well for systems which have long range interactions. From a foundational perspective, the laws of thermodynamics take on a very simple and elegant form — a class of operations and a set of statistical distances to the free state ρ_β which can never decrease. One hopes that such information theoretic laws can be used to discover a broad range of thermodynamically phenomena at the quantum level.