Steepest-Entropy-Ascent Irreversible Relaxation Towards Thermodynamic Equilibrium: the Dynamical Ansatz that Completes the Gyftopoulos-Hatsopoulos Unified Theory with a General Quantal Law of Causal Evolution[*]

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Abstract

We overview the main features of the general equation of motion that completes the Gyftopoulos-Hatsopoulos unified theory of mechanics and thermodynamics with a quantal law of causal evolution that entails relaxation towards stable equilibrium for any non-equilibrium state, no matter how far from thermodynamic equilibrium. We illustrate with numerical examples the behavior of the equation of motion by discussing spontaneous energy redistribution within an isolated, closed system composed of non-interacting identical particles with energy levels e_i and $i = 1, 2,\ldots, N$. For this system the time-dependent occupation probabilities $p_i(t)$ obey the nonlinear rate equations $\tau\, dp_i / dt = -p_i \ln p_i - \alpha(t) p_i - \beta(t) e_i p_i$ where $\alpha(t)$ and $\beta(t)$ are functions of the $p_i(t)$'s that maintain invariant the mean energy $E = \sum_{i=1}^{N} e_i p_i(t)$ and the normalization condition $1 = \sum_{i=1}^{N} p_i(t)$. The entropy $S = -k_B \sum_{i=1}^{N} p_i(t) \ln p_i(t)$ is a non-decreasing function of time until the initially nonzero occupation probabilities reach a Boltzmann-like canonical distribution over the occupied energy eigenstates. Initially zero occupation probabilities, instead, remain zero at all times. The solutions $p_i(t)$ of the rate equations are unique and well-defined for arbitrary initial conditions $p_i(0)$ and for all times, $-\infty < t < +\infty$. Existence and uniqueness both forward and backward in time allows the reconstruction of the ancestral or primordial lowest entropy state. We also illustrate the structure and main properties of the nonlinear dynamics for a composite system.

Keywords: Gyftopoulos-Hatsopoulos unified quantum theory of mechanics and thermodynamics, quantal law of causal evolution, irreversible relaxation towards stable equilibrium, ancestral or primordial lowest entropy state, existence and uniqueness both forward and backward in time, microscopic origins of entropy and irreversibility, incorporating the second law in the quantal dynamical principle.

1. Introduction

In recent years there has been a revival of interest in quantum foundational matters and nonequilibrium irreversible thermodynamics. These fields impact on an enormous applicational span. In this paper we discuss an extension of conventional quantum dynamical theory that is relevant to both fields and may prove important not only to the conceptual foundations of mechanics and thermodynamics, but also in understanding and predicting modern physics phenomena that are currently actively investigated such as decoherence, entanglement structure and dynamics in applications involving nanometric devices, fast switching times, clock synchronization, super-dense coding, quantum computation, teleportation, quantum cryptography, etc. [1] Recent discussions [2-4] have suggested possible fundamental tests of standard unitary quantum mechanics (QM), related to the existence of "spontaneous decoherence" at the microscopic level. For example, long-baseline neutrino oscillation experiments [2] might provide means of testing the existence of spontaneous decoherence and, therefore, the validity of linear

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and nonlinear extensions of standard unitary QM. As stated in Ref. [4], "recent, independent experiments [5] have provided impressive bounds on possible deviations from linear and unitary propagation of pure quantum states… But if the unitarity of pure-state propagation holds under universal conditions, one is necessarily led to a quest for genuine nonlinear extensions for isolated systems, possibly involving an explicit arrow of time. Indeed, it was pointed out in a fairly general ansatz [2, 3] that if the pure states happen to be attractors of a nonlinear evolution, then testing the unitary propagation of pure states alone cannot rule out a nonlinear propagation of mixtures."

The contemporary revival on thermodynamic foundational matters is focused on the description of the time evolution of general non-equilibrium states towards maximum-entropy stable (thermodynamic) equilibrium and is relevant to a wide variety of applications [6, 7] ranging from continuum mechanics, classical hydrodynamics, kinetic theory, quantum chemistry, molecular dynamics, non-Newtonian fluid mechanics, etc. Indeed, by general non-equilibrium states, we mean states that may be far from thermodynamic equilibrium, well beyond the usual realm of linear irreversible processes. We are concerned with the development of a well-defined time-evolution equation valid for any initial state and capable of describing entropy producing relaxation towards equilibrium by internal redistribution of energy and occupation probabilities towards a canonical or a partially canonical equilibrium distribution.

The nonlinear explicit quantum dynamical equation proposed in Ref. [8] and subsequent papers [9-15] was developed (designed) as part of a fundamental attempt to unite mechanics and thermodynamics not only at the macroscopic and mesoscopic level of description, but also at the microscopic fundamental level, without contradicting any of the successful results of standard QM. Perhaps due to technological advances towards nanometric devices, today the physical community seems more prepared to accept ideas that were viewed as heretical twenty-five years ago when the equation of motion for the unified theory was first proposed. For example, in 1984 John Maddox [16] wrote about our unified theory: "An adventurous scheme which seeks to incorporate thermodynamics into the quantum laws of motion may end arguments about the arrow of time – but only if it works." The theory has survived twenty years and in 2001 it was literally rediscovered [4, 17], at least in part, so that it appears now acceptable to postulate an extension of standard QM that assumes a "broader quantum kinematics" [18], i.e. an augmented set of true quantum states described by state operators ρ without the restriction $\rho^2 = \rho$, even for a strictly

isolated, single-particle, few-particle or single-field system, fully separable, uncorrelated, disentangled and non-interacting with its environment.

Indeed, quoting again from Ref. [4], "a physically meaningful nonlinear extension emerges when the fundamental postulates of quantum mechanics are supplemented by the first and second principles of thermodynamics, at the sole expense of ignoring the constraint of a linear, unitary evolution in time. The result is a largely irreversible, highly nonlinear generalization of the non-relativistic quantum Liouville equation, of a form closely related to the ansatz of Ref. [2] but not in the Lie-Poisson class, which features a number of rather intriguing properties. In particular, pure states still propagate unitarily into pure states according to the usual time reversible Hamiltonian dynamics."

Much work has appeared in recent years on the study of entropy-generating irreversible non-equilibrium dynamics. Limited discussions of previous work is found in Refs. [4, 17, 19] and references therein, but no thorough critical review of the subject is available, although it would be very helpful to provide proper acknowledgement of pioneering work, avoid 'rediscoveries' such as in [4] and outline the different frameworks, motivations, approaches and controversial aspects.

2. "Augmented-State-Domain" Ansatz

The fundamental ansatz that the postulates of quantum mechanics can be successfully supplemented by the first and second principles of thermodynamics by assuming a broader state domain that includes not only $\rho^2 = \rho$ but also $\rho^2 \neq \rho$ state operators, provided that the functional $-k_B \text{Tr}(\rho \ln \rho)$ is taken for the physical entropy, was first proposed (without a dynamical law) by Hatsopoulos and Gyftopoulos in a pioneering series of papers [18]. This is the first instance when this broader quantum kinematics ansatz was conceived, postulated and exploited, capitalizing on the recognition of the important role played by the stability of equilibrium in thermodynamics [20, 21], to construct a self-consistent extension of standard QM that provides a non-statistical, non-information-theoretic, micro-scopic unification of mechanics and thermodyna-mics. Again, the key ansatz is that, for any system, even if strictly isolated and uncorrelated: (1) the "true" quantum state (in the sense analogous to that of the wave function of standard quantum mechanics) is represented by a state operator ρ – a unit trace, nonnegative-definite, Hermitian operator on the Hilbert space H associated with the system according to standard QM – belonging to a "broader quantum kinematics" that includes pure

states $\left(\rho^2 = \rho\right)$ as well as non-idempotent states $\left(\rho^2 \neq \rho\right)$; and (2) the "physical" entropy (as opposed to a statistical or information-theoretic entropy related to incoherent stochastic mixtures of true states) is represented by the state functional $-k_B \mathrm{Tr}\left(\rho \ln \rho\right)$. Refs. [18, 22] give proofs that only this functional can represent the physical entropy in such a context.

Perceived as "unphysical" (by the referees of the main physics journals), the hypothesis of a state domain augmented with respect to that of traditional QM has for almost three decades been systematically rejected and substantially ignored (except for a few exceptions [23, 24]) in favor of the still prevailing approaches to dissipative quantum dynamics within the frameworks of statistical, stochastic, phenomenological, meso-scopic, information-theoretic, chaotic-behavior and bifurcation theories.

3. "Steepest-Entropy-Ascent" Ansatz

The situation did not improve when the new dynamical "steepest-entropy-ascent" ansatz was proposed and added to the scheme by the present author [8] and proved to have all the necessary mathematical features (see Section 4) to complete the Gyftopoulos-Hatsopoulos unified theory. In spite of the skeptical but encouraging editorial appearing in *Nature* that defined our scheme "adventurous" [16], the theory has continued to be ignored and rejected, mainly because its motivation appeared to be derived from theoretical reasoning only (see the recent summary in Ref. [25]).

In search for direct experimental evidence, we derived explicit solutions for a two-level system and computed the effects of the single-atom irreversible internal relaxation implied by the nonlinear equation of motion onto some basic quantum-electrodynamic results for absorption, stimulated emission, and resonance fluorescence from a single two-level atom [11, 12]. The results were obtained in the near-equilibrium linear limit and, of course, in terms of the yet undetermined internal-relaxation-time functional $\tau(\rho)$ that is part of the equation of motion. To our knowledge no one has yet attempted to verify these results experimentally and estimate or at least identify bounds on $\tau(\rho)$.

The recent and new experimental evidence of loss of quantum coherence [2, 26, 27] and the impressive effort devoted to the study of nonlinear modifications of the standard Schrödinger equation in the last twenty years [28], finally seem to make more acceptable, if not require, the Hatsopoulos-Gyftopoulos $\rho^2 \neq \rho$ augmented state domain ansatz. Five years ago, in the Addendum in which he acknowledges his oversight of our original series of papers,

Gheorghiu-Svirschevski [4] states that "Beretta's confidence in the physicality of his construction seems to find vindication after all" and "the equation of motion was derived from a variational principle which observes the principles of quantum mechanics and the fundamental laws of thermodynamics."

Provided the $\rho^2 \neq \rho$ ansatz is accepted, the proposed nonlinear equation of motion completes the dynamics and holds the promise of providing a microscopic-level explanation of the origins of entropy and irreversibility and perhaps of the recent experimental evidence of loss of quantum coherence. It is with this motivation that Ref. [4] has "re-proposed" our equation of motion together with many of its known features. Ref. [4] contributes to confirm the mathematical validity of this equation, including existence, uniqueness and positivity of solutions, and elegantly derives useful expansions and other results in the near-equilibrium linear limit. However, Ref. [4] does not rediscover the form of our nonlinear equation for a multi-component system. Nonetheless, we show in Ref. [29] that also this more general form admits of an equivalent variational formulation.

The equation of motion proposed and postulated in Refs. [8, 9] for the state operator ρ can be derived [7, 29] by means of an explicit geometrical construction that clarifies the steepest-entropy-ascent feature already recognized in Refs. [10-15]. Several new interesting additional features related to separability and fluctuations can be proved [29, 30].

The nonlinear extension of the Schrödinger equation of motion is derived, together with a full discussion of the necessary notation and definitions, in Section III of Ref. [29] for a single-component system, and in Sections X and XI of Ref. [29] for a general system consisting of *M* distinguishable component subsystems.

4. A Restrictive Set of Consistency Conditions for a Consistent Dynamical Law

The problem of deriving a well-behaved extension of Schrödinger's unitary dynamics, as is necessary if one is willing to accept the Gyftopoulos–Hatsopoulos broader quantum kinematics ansatz, has been addressed in Refs. [8, 18, 19, 31]. It amounts to defining a very demanding set of strict requirements that must be met in order for the assumed equation of motion to be consistent with both the principles of quantum mechanics and the laws of thermodynamics. The following conditions must all be satisfied [31]:

1. If the system experiences no interactions with its environment (and chemical or nuclear reactions are inhibited), energy and amounts of constituents must be conserved.

2. If the system is free, momentum conservation and Galilean invariance must be satisfied.

3. If the density operator is a projector, that is, $\rho^2 = \rho$, the evolution of ρ in time obeys the Schrödinger equation of motion, and the entropy is zero. This condition preserves all the remarkable successes of standard quantum mechanics, is consistent with experimental results, and (for projector density operators) rules out deviations from linear and unitary dynamics.

4. For isolated systems, the rate of change of the entropy functional $S(\rho) = -k_B \operatorname{Tr}\rho \ln \rho$ must be nonnegative.

5. For a system with fixed values of energy, amounts of constituents, and parameters, there must be one and only one equilibrium state for which both $d\rho/dt = 0$ and the value of the entropy is larger than that of all the other states with the same values of energy, amounts of constituents, and parameters.

6. The state of highest entropy just cited must be globally stable with respect to perturbations that do not alter the energy, the amounts of constituents and the parameters [32].

7. Onsager reciprocity relations must hold at least for nonequilibrium states in the vicinity of the highest entropy stable equilibrium states.

8. For any initial state $\rho(t_0)^\dagger = \rho(t_0) \ge \rho^2(t_0)$ and $\operatorname{Tr}\rho(t_0) = 1$, the equation of motion must admit a unique well-behaved solution $\rho(t)$ for all times, i.e., $\rho(t)$ must remain Hermitian, nonnegative and unit trace for arbitrary initial conditions.

Further conditions are given in Ref. [31], including "conservation of effective Hilbert space dimensionality" and the conditions for separability and locality that we briefly illustrate in Section 8.

As first recognized in Ref. [10], the preceding conditions are satisfied by the ansatz that the density operator evolves along a trajectory that results from the competition and coexistence of two orthogonal "forces", a Hamiltonian force that tends to drive the density operator along a unitary isentropic evolution in time and maintains constant each eigenvalue of ρ, and a conservative but dissipative force that pulls ρ towards the path of steepest entropy ascent.

5. Steepest Entropy Ascent for a Single-Component Isolated System

Here we consider only the simplest form of the general equation of motion proposed for the unified quantum theory. For convenience, we define the dimensionless entropy operator $\widetilde{S} = -B \ln \rho$, where B is the idempotent operator obtained from ρ by substituting in its spectral expansion each nonzero eigenvalue with unity.

Thus, $\widetilde{S}$ is the null operator if $\rho^2 = \rho$, and, in general, the entropy functional $-k_B \operatorname{Tr}\rho \ln \rho$ can be written as $k_B \operatorname{Tr}\rho \widetilde{S}$.

For a single isolated constituent without non-Hamiltonian time-invariants, it is only for the zero entropy states ($\rho^2 = \rho$) that the postulated nonlinear equation of motion coincides with the Schrödinger unitary dynamics of standard quantum mechanics, i.e.,

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] \qquad (1)$$

For an arbitrary nonzero entropy state ($\rho > \rho^2$), it is instead given by the relation

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] - \frac{1}{\tau}D \qquad (2)$$

where τ is a scalar time constant or functional, D is a nonlinear operator function of ρ, $\widetilde{S}$, H defined by any of the following equivalent forms

$$D = -\frac{\begin{vmatrix} \frac{1}{2}\{\widetilde{S}, \rho\} & \rho & \frac{1}{2}\{H, \rho\} \\ \operatorname{Tr}\rho\widetilde{S} & 1 & \operatorname{Tr}\rho H \\ \operatorname{Tr}\rho H\widetilde{S} & \operatorname{Tr}\rho H & \operatorname{Tr}\rho H^2 \end{vmatrix}}{\begin{vmatrix} 1 & \operatorname{Tr}\rho H \\ \operatorname{Tr}\rho H & \operatorname{Tr}\rho H^2 \end{vmatrix}}$$

$$= \frac{\begin{vmatrix} \rho \ln \rho & \rho & \frac{1}{2}\{H, \rho\} \\ \operatorname{Tr}\rho \ln \rho & 1 & \operatorname{Tr}\rho H \\ \operatorname{Tr}\rho H \ln \rho & \operatorname{Tr}\rho H & \operatorname{Tr}\rho H^2 \end{vmatrix}}{(\Delta H)^2}$$

$$= -\frac{1}{2}\{\widetilde{S}, \rho\} + \alpha(\rho)\rho + \beta(\rho)\frac{1}{2}\{H, \rho\} \qquad (3)$$

where $|\cdot|$ denotes a determinant, the operators $\widetilde{S}$ and ρ commute so that $(1/2)\{\widetilde{S}, \rho\} = -\rho \ln \rho$, and $\alpha(\rho)$ and $\beta(\rho)$ are the nonlinear functionals

$$\alpha(\rho) = \operatorname{Tr}\rho\widetilde{S} - \beta\operatorname{Tr}\rho H \qquad (4)$$

$$\beta(\rho) = \frac{\operatorname{Tr}\rho\widetilde{S}H - \operatorname{Tr}\rho\widetilde{S}\operatorname{Tr}\rho H}{\operatorname{Tr}\rho H^2 - (\operatorname{Tr}\rho H)^2} \qquad (5)$$

Eq. (2) satisfies all the consistency conditions listed in Section 4. For example, it is easy to verify that

$$\frac{d}{dt}\operatorname{Tr}\rho = \operatorname{Tr}\frac{d\rho}{dt} = \operatorname{Tr}D = 0 \qquad (6)$$

$$\frac{d}{dt}\operatorname{Tr}\rho H = \operatorname{Tr}\frac{d\rho}{dt}H = \operatorname{Tr}DH = 0 \qquad (7)$$

$$\frac{d}{dt}\operatorname{Tr}\rho\widetilde{S} = \operatorname{Tr}\frac{d\rho}{dt}\widetilde{S} = \operatorname{Tr}D\widetilde{S} \ge 0 \qquad (8)$$

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In addition, it can be shown that if $\rho > \rho^2$ at one time, it remains so at all times, both forward and backward in time. The only equilibrium density operators that are stable according to this dynamics are the highest entropy operators in the one parameter family

$$\rho^{se} = \frac{\exp(-H/k_B T)}{\text{Tr}\exp(-H/k_B T)} \qquad (9)$$

where the parameter T is readily identified with the temperature (as defined in Refs. [18, 21]).

Proofs of these and other intriguing features of Eq. (2) and its more general forms are given in Refs. [4, 7, 10–15, 29]. In particular, the form of the equation can be readily generalized to include other *generators of the motion* in addition to the Hamiltonian operator H, such as the number-of-particle operators N_i for systems that at stable equilibrium are described by the grand canonical density operator

$$\rho^{se} = \frac{\exp\left[-\left(H - \sum \mu_i N_i\right)/k_B T\right]}{\text{Tr}\exp\left[-\left(H - \sum \mu_i N_i\right)/k_B T\right]} \qquad (10)$$

Unitary dynamics (Eq. (1)) applied to nonzero entropy states ($\rho > \rho^2$) would maintain time-invariant each of the eigenvalues of ρ. Instead, Eq. (2) maintains invariant only the initially zero eigenvalues of ρ and, therefore, conserves the cardinality of the set of zero eigenvalues, dim Ker(ρ) = const. This important feature implies that if the isolated system is prepared in a state that does not require all the eigenvectors $|\psi_\ell\rangle$ of H so that $\rho(0)|\psi_\ell\rangle = 0$ for some values of ℓ, then the zero eigenvalues persist at all times, that is, $\rho(t)|\psi_\ell\rangle = 0$. This is the nontrivial condition that we call conservation of effective Hilbert space dimensionality (by effective Hilbert space we mean the range Ran ρ of the density operator, namely the subspace of $\mathbb{H}$ spanned by the eigenvectors of ρ with nonzero eigenvalues). It can be viewed as an extension of item (3) of the consistency conditions listed in Section 4 and, of course, it is a characteristic feature of all successful models and theories of the physics of isolated systems.

The non-Hamiltonian dissipative term $-D/\tau$ in Eq. (2) pulls the state operator in the direction of the projection of the gradient of the entropy functional $k_B \text{Tr}\rho\widetilde{S}$ onto the (hyper) plane of constant $\text{Tr}\rho$ and $\text{Tr}\rho H$. Because the system is isolated, the entropy ceases to increase only when the largest entropy value is reached consistent with the specified dimensionality of the Hilbert space. The same would hold for adiabatic processes described by a time-dependent H.

As recently shown in Refs. [4, 29], the steepest-entropy-ascent feature is confirmed also by a variational formulation wherein the form (3)

of the dissipative term in Eq. (2) is obtained as a result of searching among all possible directions in which operator ρ can change with the direction of maximal entropy generation compatible with the constraints that ρ remains a well-defined operator, and $\text{Tr}\rho$ and $\text{Tr}\rho H$ remain time invariant. For the more general form that conserves also other observables in addition to the energy see Ref. [29].

Given any initial density operator, it is possible to solve the equation of motion not only in forward time but also in backward time [7, 11] and reconstruct the entire trajectory in ρ space for $-\infty < t < +\infty$, provided of course either the Hamiltonian H is time independent or its dependence on time is well behaved at all times.

In Ref. [12], Eq. (2) is applied to study atomic relaxation in a two-level atom. By modeling the interaction between a single two-level atom and the quantum electromagnetic field that corresponds to driving the two-level atom near resonance by a nearly monochromatic laser beam, it is shown that the nonlinear irreversible atomic relaxation described by the term $-D/\tau$ in Eq. (2) implies corrections to the resonance fluorescence, absorption and stimulated emission line shapes. Such experiments on properly prepared homogeneous ensembles that require $\rho \neq \rho^2$ would provide experimental evidence and a means to evaluate the atomic relaxation time τ.

6. One Particle Approximation for a Boltzmann Gas

As an illustration of the applications of Eq. (2), we consider an isolated system composed of a single-component gas of non-interacting identical particles with single-particle energy eigenvalues e_i for $i = 1, 2, \ldots, N$ where N is finite and the e_i's are repeated in case of degeneracy. As done in Ref. [7], we restrict for simplicity our analysis to the class of dilute-Boltzmann-gas states in which the particles are independently distributed among the N (possibly degenerate) one-particle energy eigenstates. In density operator language, this is tantamount to restricting the analysis to the subset of one-particle density operators ρ that are diagonal in the representation in which also the one-particle Hamiltonian operator H is diagonal $([H, \rho] = 0)$. We denote by p_i the probability of the i-th energy eigenstate, so that the per-particle energy and entropy functionals are given by the relations

$$E = \sum_{i=1}^{N} e_i p_i \quad S = -k_B \sum_{i=1}^{N} p_i \ln p_i \quad \sum_{i=1}^{N} p_i = 1 \quad (11)$$

The nonlinear equation of motion maintains the initially zero probabilities equal to zero, whereas the rates of change of the nonzero probabilities, for $i, j = 1, 2, \ldots, N$, are given by

$$\frac{dp_j}{dt} = -\frac{1}{\tau} \frac{\begin{vmatrix} p_j \ln p_j & p_j & e_j p_j \\ \sum p_i \ln p_i & 1 & \sum e_i p_i \\ \sum e_i \ln p_i & \sum e_i p_i & \sum e_i^2 p_i \end{vmatrix}}{\begin{vmatrix} 1 & \sum e_i p_i \\ \sum e_i p_i & \sum e_i^2 p_i \end{vmatrix}} \quad (12)$$

The solutions of these equations are well-behaved in the sense that they satisfy all the conditions listed in Section 4. In particular, as exemplified by the numerical simulations discussed in Section 7, they exhibit the following general features:

1. They conserve the energy and trace of ρ.

2. They preserve the non-negativity of each p_i.

3. The maintain the rate of entropy generation non-negative.

4. They maintain the dimensionality of the effective Hilbert space, that is, for a density operator ρ with $[H,\rho] = 0$ and eigenvalues $\boldsymbol{p}$ given by any set of p_i's, they maintain invariant the vector $\boldsymbol{\delta}(\boldsymbol{p})$ of δ_i's defined so that for each $i = 1,2,...,N$, $\delta_i = 1$ if $p_i \neq 0$ and $\delta_i = 0$ if $p_i = 0$.

5. They drive any arbitrary initial density operator $\rho(t_o)$ towards the partially canonical (or canonical if $\delta_i = 1$ for all energy eigenstates of the Boltzmann gas) equilibrium density operator $\rho(+\infty)$ with time-independent eigenvalues $\boldsymbol{p}(+\infty)$ in the energy representation given by

$$p_j^{pe}(E, \boldsymbol{\delta}) = \frac{\delta_j \exp(-\beta^{pe}(E,\boldsymbol{\delta}) e_j)}{\sum_{i=1}^N \delta_i \exp(-\beta^{pe}(E,\boldsymbol{\delta}) e_i)} \quad (13)$$

where $\boldsymbol{\delta} = \boldsymbol{\delta}(\boldsymbol{p}(0))$, the value of β^{pe} is determined by the initial condition $\sum_{i=1}^N e_i p_{p_i}^{pe}(E,\boldsymbol{\delta}) = E = E(\boldsymbol{p}(0))$, and the superscript "pe" is used to indicate that the system is in an unstable or, so-called, partial equilibrium state.

Among all the equilibrium states just cited, there exists one and only one that is stable (superscript "se") and corresponds to the largest value of the entropy for the given value of energy E and for which the eigenvalues of the density operator in the energy representation are given by the canonical distribution

$$p_j^{se}(E) = \frac{\exp(-e_j/kT(E))}{\sum_{i=1}^N \exp(-e_i/kT(E))} \quad (14)$$

where $T(E)$ may be shown to be equal to the derivative of the energy with respect to the entropy for the stable equilibrium states of the Boltzmann gas. By de-finition, the derivative just cited is the temperature.

For a general non-equilibrium state, the rate of entropy generation may be written as a ratio of Gram determinants in the form

$$\frac{\tau}{k_B}\frac{dS}{dt} = \frac{\begin{vmatrix} \sum p_i(\ln p_i)^2 & \sum p_i \ln p_i & \sum e_i p_i \ln p_i \\ \sum p_i \ln p_i & 1 & \sum e_i p_i \\ \sum e_i p_i \ln p_i & \sum e_i p_i & \sum e_i^2 p_i \end{vmatrix}}{\begin{vmatrix} 1 & \sum e_i p_i \\ \sum e_i p_i & \sum e_i^2 p_i \end{vmatrix}}$$

$$(15)$$

and its non-negativity follows from the well-known properties of Gram determinants.

Given any initial density operator, it is possible to solve the equation of motion for all values of time, that is $-\infty < t < +\infty$. In the limit as $t \to +\infty$, the trajectory approaches a largest entropy equilibrium state with a density operator that is canonical over the energy eigenstates initially included in the analysis. An exception to this conclusion is the case of the initial density operator being a projector $\rho = \rho^2$. Then the evolution in time follows the Schrödinger equation and is unitary and reversible, except if the projector is an energy eigenprojector which is stationary.

7. Numerical Simulations

The energy versus entropy diagram introduced by Gibbs represents the intersection with the E–S plane of the E–S–V–$\boldsymbol{n}$ surface representing the stable thermodynamic equilibrium states of a system, assuming that the energy eigenvalues depend on the volume V and the amounts of constituents $\boldsymbol{n}$, so that the surface is represented by the so-called fundamental relation $S = S(E, \{e_j(V,\boldsymbol{n})\})$. In [21] the use of such a diagram has been extended to include the projection onto the E–S plane of all other states, i.e., not only the stable equilibrium states but also the non-equilibrium and the non-stable equilibrium states, with given fixed values of V and $\boldsymbol{n}$ and, therefore, a given fixed set of energy eigenvalues. On such a diagram, therefore, one point represents in general a multitude of distributions, except at every point of maximal entropy for each given value of E (V and $\boldsymbol{n}$ are fixed) which corresponds to a unique canonical distribution (Eq. (14)), i.e., a unique stable thermodynamic equilibrium state.

For a four-level, non-degenerate system, Figure 1 presents the families of possible canonical (Eq. (14)) and partially-canonical (Eq. (13)) equilibrium distributions which in our dynamics are the only ones with zero entropy generation rate. We recall that the slope of these curves is related to the parameter $\beta^{pe}(E,\boldsymbol{\delta})$ because $\partial S^{pe}(E,\boldsymbol{\delta})/\partial E|_{\boldsymbol{\delta}} = k_B \beta^{pe}(E,\boldsymbol{\delta})$, which for the canonical distribution (all δ_i's equal to unity) is $\partial S(E)/\partial E = k_B \beta(E) = 1/T(E)$.

The number of possible distributions that share a given pair of values of E and S is in

general a (N-3)–fold infinity except at maximum entropy for each value of E, where the distribution is unique and at a few other notable exceptions such as at minimal entropy for each given E where the distribution may be unique or sometimes manyfold.

The next figures show typical time dependences of the occupation probabilities that result from the numerical integration (by means of a standard
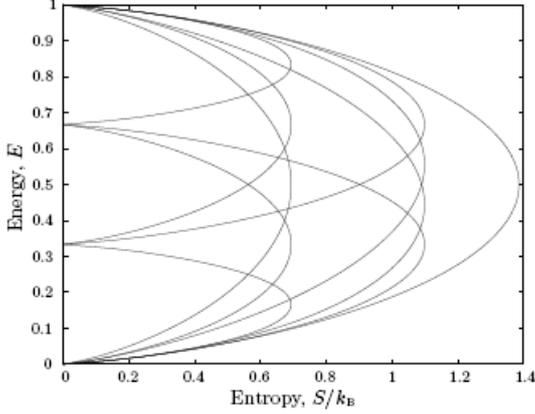
Figure 1: From Ref. [7]. Representation on an energy versus entropy diagram (for N=4 and non-degenerate eigenstates with energies $\boldsymbol{e}$ = [0, 1/3, 2/3, 1]) of the families of possible canonical and partially-canonical equilibrium distributions which in our dynamics are the only ones with a zero entropy generation rate. For example, a horizontal line at E = 0.4 intersects seven different families of partially canonical states.

Runge-Kutta algorithm) of Eq. (12) both forward and backward in time. All trajectories in these figures refer to a system with N=4 and non-degenerate eigenstates with $\boldsymbol{e}$ = [0, 1/3, 2/3, 1] and all have the same mean energy E = 2/5; they all tend, of course, to the canonical distribution $\boldsymbol{p}^{se}(2/5)$ = [0.3474, 0.2722, 0.2133, 0.1671] that has inverse temperature $\beta^{se}(2/5)$ = 0.7321. They are obtained by assuming for all cases an initial distribution $\boldsymbol{p}(0)$ obtained by perturbing the canonical distribution $\boldsymbol{p}^{se}(E)$ (Eq. (14)) according to

$$\widetilde{p}_j = \frac{f_j p_j^{se}(E)}{\sum_{i=1}^N f_i p_i^{se}(E)} \qquad (16)$$

with the energy preserving perturbing factors defined as follows for $j = 1,2,\ldots,N$:

$$f_j = 1 - \lambda + \lambda \frac{p_j^{pe}(E,\boldsymbol{\delta})}{p_j^{se}(E)} \quad \text{with } 0 < \lambda < 1 \quad (17)$$

where λ is otherwise arbitrary and also $\boldsymbol{\delta}$ is arbitrarily chosen among the possible vectors of 0's and 1's compatible with the given value of E and Eq. (13) of the distribution $\boldsymbol{p}^{pe}(E,\boldsymbol{\delta})$ (see Figure 1), where $\beta^{pe}(E,\boldsymbol{\delta})$ is computed by

solving the equation $\sum_i p_i^{pe}(E,\boldsymbol{\delta})e_i = E$. For all subsequent figures, we use $\lambda = 0.9$.

Figure 2 shows the time dependence of the occupation probabilities that results under the assumptions just cited using E =2/5, λ =0.9 and $\boldsymbol{\delta}$ = [1, 1, 0, 1] in Eq. (17) and subsequently substituting into Eqs. (16), that is,

$$\boldsymbol{p}(0) = \lambda\, \boldsymbol{p}^{pe}(E,\boldsymbol{\delta}) + (1-\lambda)\boldsymbol{p}^{se}(E) \qquad (18)$$
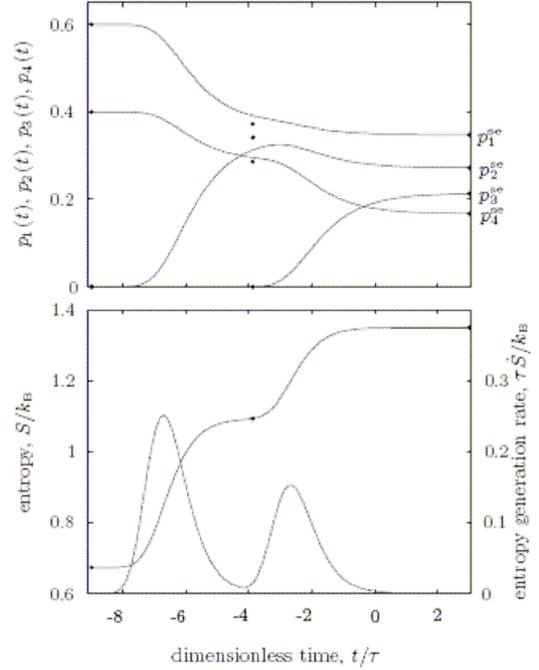
Figure 2: From Ref. [7]. Top: typical time dependences of the occupation probabilities that result from the numerical integration of Eq. (12) both forward and backward in time for N = 4, $\boldsymbol{e}$ = [0,1/3,2/3,1], energy E = 2/5, initial state at $t = 0$ from Eq. (18) with $\lambda = 0.9$ and $\boldsymbol{\delta} = [1,1,0,1]$. The dots on the right represent the maximum entropy distribution; the dots at the left represent the lowest-entropy or 'primordial' distribution; the dots in the middle represent the $\boldsymbol{p}^{pe}(E,\boldsymbol{\delta})$ distribution used in Eq. (18) to select the $t = 0$ state, plotted at the instant in time when the entropy of the time-varying trajectory is equal to the entropy of the $\boldsymbol{p}^{pe}(E,\boldsymbol{\delta})$ distribution. Bottom: the corresponding time dependence of the entropy (left axis) and the entropy generation rate (right axis).

It is noteworthy that when the trajectory gets very close to the partially-canonical unstable-equilibrium distribution $\boldsymbol{p}^{pe}(E=2/5)$, $\boldsymbol{\delta}$ = [1, 1, 0, 1], the entropy surface presents a local 'plateau', and the entropy generation rate drops almost to zero, but shortly thereafter, the trajectory bends in a direction of steeper slope that drives the generation up again until the canonical distribution $\boldsymbol{p}^{se}(E)$ = [0.3474, 0.2722, 0.2133, 0.1671] is finally approached with the inverse temperature $\beta^{se}(2/5)$ = 0.7321. Of course, the entropy is a

monotonically increasing function of time along the entire trajectory.

Figure 3 shows the same trajectory as well as six other trajectories; but instead of plotting the time dependence of the occupation probabilities, we plot them against the entropy. The initial (time $t = 0$) distribution used to obtain these seven sample trajectories are obtained from Eq. (18) with $E = 2/5$, $\lambda = 0.9$ and each of the seven partially ca-
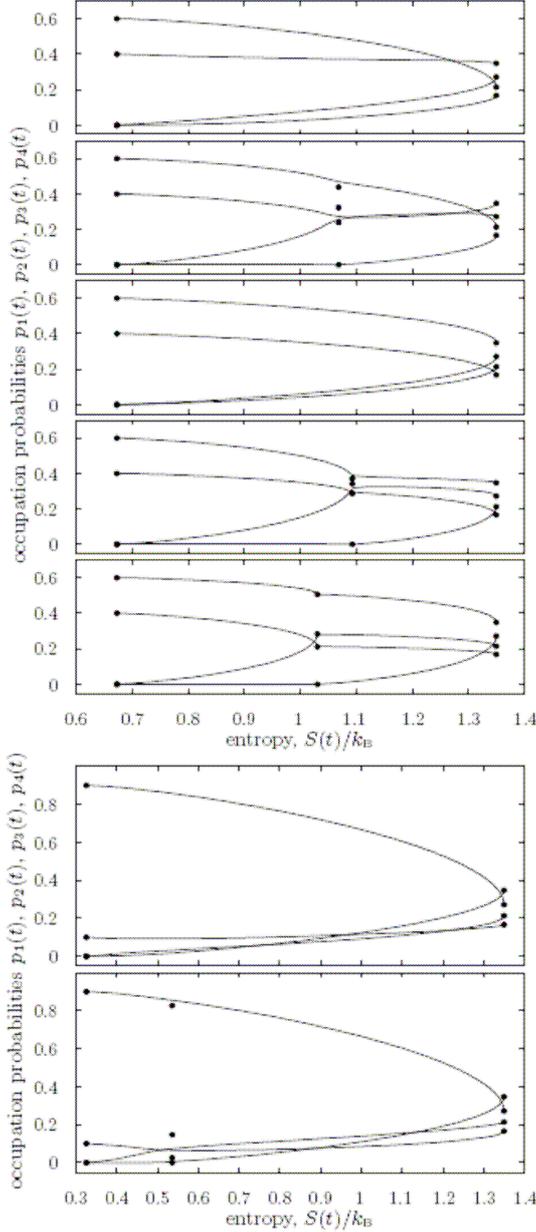
Figure 3: From Ref. [7]. Plots of $p_i(t)$ versus $S(t)$ for seven sample time dependences of the occupation probabilities that result from the numerical integration of Eq. (12) both forward and backward in time, for different initial distributions.

nonical states corresponding to the given value of the energy. These seven states are easily identified on the E–S diagram in Figure 1 by drawing a

horizontal line at $E = 0.4$. For the first, third, and sixth trajectories, we use the $p^{pe}(E, \delta)$ states with $\delta = [1, 0, 1, 0]$, $\delta = [1, 0, 0, 1]$ and $\delta = [0, 1, 0, 1]$, respectively, which (as is apparent from the subsequent Figure 4) are the lowest-entropy boundary points of the entropy surface for the given energy, and turn out also to be the 'primordial' states of the corresponding trajectories. For the remaining trajectories, we use the $p^{pe}(E, \delta)$ states with $\delta = [1, 1, 1, 0]$, $\delta = [1, 1, 0, 1]$, $\delta = [1, 0, 1, 1]$, and $\delta = [0, 1, 1, 1]$, respectively. These too are boundary points of the entropy surface, but they correspond to partial maxima (over the subset of distributions with one unoccupied eigenstate as specified by the corresponding zero element of δ). It is seen that these partial maxima affect the trajectories passing nearby by acting as partial attractors especially in the initial phase of the time evolution.

Figure 4 is a more elaborate representation of the same seven trajectories. They are shown four times from different perspectives on the background of contour plots of the entropy surface, for four pairs of occupation probabilities. Indeed, for $N = 4$ and fixed energy E, the number
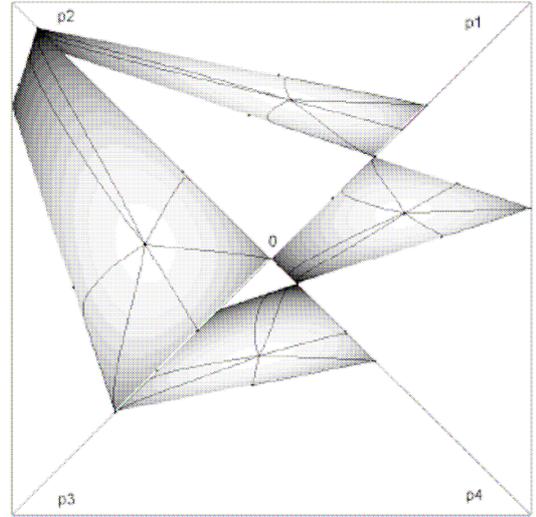
Figure 4: From Ref. [7]. Each rotated quadrant of the graph represents, for the corresponding pair of occupation probabilities, a plot of the seven trajectories shown in Figure 3 drawn over contour plots of the entropy surface.

of independent occupation probabilities is two. Thus, for four pairs of probabilities ($p_1 - p_2$, $p_2 - p_3$, $p_3 - p_4$, $p_4 - p_1$), we draw the contour plot of the entropy surface over the entire domain of allowed values (which, of course, are contained in a triangular region of the first quadrant), and over this plot we draw the seven trajectories (and the seven partially canonical states used to choose them). To save space, we then rotate each of the four graphs (respectively,

by 45, 135, 225, 315 degrees) and present them in the same figure (Figure 4). The figure visualizes clearly that the trajectories indeed follow paths of locally-steepest-entropy-ascent and also unfold smoothly backward in time to the 'primordial' states. We also note that these lowest-entropy states exhibit a singular behavior in that, for example, state [2/5, 0, 3/5, 0] is the primordial state for two entirely different trajectories, state [3/5, 0, 0, 2/5] for three others, and state [0, 9/10, 0, 1/10] for the remaining two. Moreover, the partially canonical states appear as partial attractors of trajectories passing nearby, as seen quite clearly for the second, fourth and fifth trajectories of Figure 3, which are partially attracted by the partially canonical states with δ = [1, 1, 1, 0], δ = [1, 1, 0, 1] and δ = [1, 0, 1, 1], respectively.

8. Composite System Dynamics

As in standard quantum theory, the composition of a system is embedded in the structure of the associated Hilbert space as a direct product of the subspaces associated with the individual elementary constituent subsystem, as well as in the form of the Hamiltonian operator.

For simplicity, we consider here a system composed of two distinguishable and indivisible elementary constituent subsystems. For example, each subsystem may be a different elementary particle or a Fermi-Dirac or Bose-Einstein or Boltzmann field (in which case the corresponding Hilbert space is a Fock space). The subdivision into elementary constituents, each considered as indivisible, is reflected by the structure of the Hilbert space H as a direct product of subspaces,

$$\mathsf{H} = \mathsf{H}^A \otimes \mathsf{H}^B \qquad (19)$$

and is particularly important because it defines the level of description of the system and specifies its elementary structure together with the Hamiltonian operator

$$H = H_A \otimes I_B + I_A \otimes H_B + V \qquad (20)$$

where H_J is the Hamiltonian operator on H^J associated with subsystem J when isolated, for J=A,B, and V (on H) is the interaction Hamiltonian among the two subsystems.

The specification just cited determines also the structure of the nonlinear dynamical law, which is different depending on whether the system is or is not sub-divisible into indivisible subsystems, i.e., whether or not it has an internal structure. The dependence of the structure of the dynamical law on the level of description of the system's internal structure in terms of elementary indivisible constituents is an important consequence of having given up linearity [15, 29].

In the simplest case that we are considering

here, the dissipative term in the equation of motion is a function of two novel important nonlinear local observables that we call "locally perceived overall-system energy" and "locally perceived overall-system entropy" that represent measures of how the overall-system energy and entropy operators, H and $\tilde{S} = -B \ln \rho$, are "felt" locally within the Jth subsystem [9, 29]. They are associated with the following local operators:

$$(H)^J = \mathrm{Tr}_{\bar{J}}\left[(I_J \otimes \rho_{\bar{J}})H\right] \qquad (21)$$

$$(\tilde{S})^J = \mathrm{Tr}_{\bar{J}}\left[(I_J \otimes \rho_{\bar{J}})\tilde{S}\right] \qquad (22)$$

where J = A, B and $\bar{J}$ =B, A, $\rho_J = \mathrm{Tr}_{\bar{J}}\rho$ and $\rho_{\bar{J}} = \mathrm{Tr}_J \rho$.

Operator $\tilde{S}_J$ may be interpreted as the subsystem entropy operator only if subsystem J is not correlated with the other subsystem, i.e., only if ρ can be written as

$$\rho = \rho_A \otimes \rho_B \qquad (23)$$

then the subsystem entropy is defined and given by the nonlinear state functional of the reduced state operator $k_B \mathrm{Tr}_J \rho_J \tilde{S}_J = -k_B \mathrm{Tr}_J \rho_J \ln \rho_J$, and $\tilde{S} = \tilde{S}_A \otimes I_B + I_A \otimes \tilde{S}_B$. If the subsystems are correlated, then no individual entropies can be defined; however, the functional $k_B \mathrm{Tr}_J \rho_J (\tilde{S})^J$ is always well-defined and may be interpreted as the subsystem's local perception of the overall-system entropy.

Similarly, energy is defined for subsystem J only if it is not interacting with the other subsystem, i.e., if H can be written as

$$H = H_A \otimes I_B + I_A \otimes H_B \qquad (24)$$

Then the energy of J is given by the functional. $\mathrm{Tr}_J \rho_J H_J$. The functional $\mathrm{Tr}_J \rho_J (H)^J$ instead is always well-defined, even if the subsystems are interacting, and may be interpreted as the subsystem's local perception of the overall-system energy.

In order for an equation of motion of quantum thermodynamics to be acceptable for both the description of the time evolution of a composite system and the exclusion of non-locality paradoxes such as faster-than-light communication, the following conditions must be added to the list of Section 4 [31]:

1. For a system composed of non-interacting subsystems, the energy of each subsystem, $\mathrm{Tr}_J \rho_J H_J$, must be time invariant (separate energy conservation).

2. For a system composed of subsystems in independent states, that is, such that $\rho = \rho_A \otimes \rho_B$, the entropy of each subsystem J, $k \mathrm{Tr}_J \rho_J \tilde{S}_J$, must be non-decreasing in time (separate entropy non-

decrease).

3. Non-interacting subsystems that are initially in correlated states must be unable to influence each other's time evolution as long as they remain non-interacting, even if each of them separately interacts with other systems.

For an isolated composite of r constituents without non-Hamiltonian time-invariants, the postulated nonlinear equation of motion coincides with Eq. (1) only for zero entropy states $\left(\rho^2 = \rho\right)$, whereas for an arbitrary nonzero entropy state $\left(\rho^2 < \rho\right)$ the equation of motion is

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H,\rho] - \frac{1}{\tau_A}D_A \otimes \rho_B - \frac{1}{\tau_B}\rho_A \otimes D_B \quad (25)$$

where each D_J is the nonlinear operator defined by the relations

$$D_J = -\frac{1}{2}\left\{\left(\widetilde{S}\right)^J, \rho_J\right\} - \alpha_J \rho_J + \beta_J \frac{1}{2}\left\{(H)^J, \rho_J\right\} \quad (26)$$

$$\alpha_J = -\mathrm{Tr}_J \rho_J \left(\widetilde{S}\right)^J + \beta_J \mathrm{Tr}_J \rho_J (H)^J \quad (27)$$

$$\beta_J = \frac{\mathrm{Tr}_J \rho_J \frac{1}{2}\left\{\left(\widetilde{S}\right)^J, (H)^J\right\} - \mathrm{Tr}_J \rho_J \left(\widetilde{S}\right)^J \mathrm{Tr}_J \rho_J (H)^J}{\mathrm{Tr}_J \rho_J (H)^J (H)^J - \left[\mathrm{Tr}_J \rho_J (H)^J\right]^2} \quad (28)$$

It is noteworthy that the functional dependence of each D_J on ρ_J, $\left(\widetilde{S}\right)^J$, $(H)^J$ is the same as that of D on ρ, S, and H for the single constituent system (Eq. (3)). Proofs that Eq. (25) satisfies all the consistency conditions listed in Section 4 plus the three just cited are given in Refs. [8, 9, 29]. Again, it is easy to verify that

$$\mathrm{Tr}_J D_J = 0 \quad \mathrm{Tr}_J D_J (H)^J = 0 \quad \mathrm{Tr}_J D_J \left(\widetilde{S}\right)^J \geq 0 \quad (29)$$

and, therefore,

$$\frac{d}{dt}\mathrm{Tr}\rho = \mathrm{Tr}_A D_A + \mathrm{Tr}_B D_B = 0 \quad (30)$$

$$\frac{d}{dt}\mathrm{Tr}\rho H = \mathrm{Tr}_A D_A (H)^A + \mathrm{Tr}_B D_B (H)^B = 0 \quad (31)$$

$$\frac{d}{dt}\mathrm{Tr}\rho\widetilde{S} = \mathrm{Tr}_A D_A \left(\widetilde{S}\right)^A + \mathrm{Tr}_B D_B \left(\widetilde{S}\right)^B \geq 0 \quad (32)$$

Finally, it is shown that if $\rho^2 < \rho$ at one time, it remains so at all times, that is, for $-\infty < t < +\infty$.

By taking the partial trace of $d\rho/dt$ (as given by Eq. (25)) over H^B, we obtain the rate of change of the reduced state operator of subsystem A, i.e., $d\rho_A/dt = \mathrm{Tr}_B d\rho/dt$. If B is not interacting with A, i.e., the Hamiltonian is given

by Eq. (24) with $V = 0$, $d\rho_A/dt$ turns out to be independent of H_B. This means that it is impossible to affect the local observables of A by acting only on B, and so non-locality paradoxes are excluded by the novel equation of motion. This, however, does not mean that existing entanglement and/or correlations between A and B established by past interactions that have been subsequently turned off have no influence whatsoever on the time evolution of the local observables of either A or B. In particular, there is no physical reason to expect that two different density operators ρ and ρ' such that $\rho'_A = \rho_A$ should evolve with identical local dynamics $(d\rho'_A/dt = d\rho_A/dt)$ whenever A does not interact with B, because the fact that $\rho \neq \rho'$ means that in these two states the subsystems are differently correlated and/or entangled and, therefore, the two local evolutions should in general be different, at least until memory of the entanglement and the correlations established by turned-off past interactions have faded away (spontaneous decoherence) as a consequence of the irreversible entropy-increasing evolution [31]. This subtlety is also captured by the novel equation of motion. Indeed, $d\rho_A/dt$ in general depends not only on the "local" reduced density operator ρ_A but also on the overall density operator ρ through operator $\left(\widetilde{S}\right)^A = \left(-B\ln\rho\right)^A$, resulting in a collective behavior effect on the local dynamics that originates from the existing residual correlations due to past interactions.

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