

WELL-BEHAVED NONLINEAR EVOLUTION EQUATION FOR STEEPEST-ENTROPY-ASCENT DISSIPATIVE QUANTUM DYNAMICS

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NOT ONLY IT CAN BE USED AS AN ALTERNATIVE TO LINDBLAD-FORM LINEAR MODEL EQUATIONS FOR REDUCED QUANTUM DYNAMICS ...

1 Introduction

Much work has appeared in recent years on the study of entropy-generating irreversible nonequilibrium dynamics. Limited discussions of previous work is found in [1, 2, 3, 4] 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 ‘re-discoveries’ such as in [5] and outline the different frameworks, motivations, approaches and controversial and interpretational aspects (e.g., for pioneering contributions see [6, 7, 8]).

To be sure, recent discussions (see e.g. [2, 5, 9, 10]) on possible fundamental tests of standard unitary quantum mechanics, related to the existence of ‘spontaneous decoherence’ at the microscopic level, and on understanding and predicting decoherence in important future applications [11] involving nanometric devices, fast switching times, clock synchronization, superdense coding, quantum computation, teleportation, quantum cryptography, etc. show that the subject of irreversible nonequilibrium dynamics is by no means settled.

In this paper, we outline the main features of the nonlinear quantum evolution equation proposed by the author [12]–[19]. Such equation may be used as a model (Sections 2–4) of reduced subsystem dynamics to complement various historical and contemporary efforts to extend linear Markovian theories of dissipative phenomena and relaxation based on master equations, Lindblad and Langevin equations, to the nonlinear and far nonequilibrium domain. It may also be used as the fundamental dynamical principle (Section 5) in theories that attempt to unite mechanics and thermodynamics, such as the Hatsopoulos-Gyftopoulos unified theory [8] which motivated the original development of this well-behaved general nonlinear equation for the density operator.

2 General class of nonlinear evolution equations for non-Lindblad dissipative quantum dynamics

Let \mathcal{H} ($\dim \mathcal{H} \leq \infty$) be the Hilbert space and H the Hamiltonian operator associated with a system in standard Quantum Mechanics. We assume that the quantum states are one-to-one with the linear hermitian operators ρ on \mathcal{H} with $\text{Tr}(\rho) = 1$ and $\rho \geq \rho^2$, and we assume a dynamical equation of the form [12]–[19]

$$\frac{d\rho}{dt} = \rho E(\rho) + E^\dagger(\rho) \rho, \quad (1)$$

where $E(\rho)$ is an operator-valued function of ρ that we may call the ‘evolution’ operator and in general is non-hermitian. Without loss of generality, we write $E = E_+ + iE_-$ where $E_+ = (E + E^\dagger)/2$ and $E_- = (E - E^\dagger)/2i$ are hermitian operators that, for convenience, we rename as $\Delta M(\rho)/(2k_B\tau\rho)$ and H/\hbar , respectively, so that Eq. (1) takes the form [18, 19]

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] + \frac{1}{2k_B\tau\rho}(\Delta M(\rho), \rho), \quad (2)$$

where $\{ \cdot, \cdot \}$ and $\{ \cdot, \cdot \}$ are the usual commutator and anti-commutator, H (assumed independent of ρ , but not necessarily independent of time t) is identified with the Hamiltonian operator, \hbar the reduced Planck constant, k_B the Boltzmann constant; moreover, $\Delta M(\rho)$ is a hermitian operator-valued, possibly nonlinear function of ρ which, together with the positive definite, possibly nonlinear functional $\tau(\rho)$ of ρ , describes the dissipative dynamics of the system, and is such that $\text{Tr}[\rho\Delta M(\rho)] = 0$ as required to preserve ρ unit trace.

The reason for considering a dynamical law of the form (2) is that the explicit expression of $\Delta M(\rho)$ that generates steepest-entropy-ascent (maximal entropy generation) conservative dynamics of an isolated system compatible with all thermodynamics requirements [4] is known [12]–[19].

The steepest-entropy-ascent form of the operator function $\Delta M(\rho)$ is defined in Section 3 in terms of the operator [17, 18, 19]

$$M(\rho) = S(\rho) - \frac{H}{\theta(\rho)} + \frac{\mu(\rho) \cdot \mathbf{N}}{\theta(\rho)}, \quad (3)$$

where $S(\rho)$ is the entropy operator [precise definition in Eq. (15)], and the functionals $\theta(\rho)$ and $\mu(\rho)$ are defined in Section 3, Eqs. (16)–(19)]. We call operator $M(\rho)$ the *generalized nonequilibrium Massieu-function operator*, because at thermodynamic equilibrium its mean value belongs to the family of entropic characteristic functions introduced by Massieu [20], i.e.,

$$\langle M \rangle_c = \langle S \rangle_c - \frac{\langle H \rangle_c}{T} + \frac{\mu \cdot \langle \mathbf{N} \rangle_c}{T}, \quad (4)$$

where $\langle S \rangle_c$, $\langle H \rangle_c$, $\langle \mathbf{N} \rangle_c$, T and μ are the equilibrium entropy, energy, amounts of constituents, temperature and chemical potentials, respectively.

We consider the space $\mathcal{L}(\mathcal{H})$ of linear operators on \mathcal{H} equipped with the real scalar product

$$\langle F|G \rangle = \text{Tr}(F^\dagger G + G^\dagger F)/2 = \langle G|F \rangle, \quad (5)$$

and the real antisymmetric bilinear form

$$\langle F|G \rangle = i \text{Tr}(F^\dagger G - G^\dagger F)/2 = -\langle G|F \rangle = \langle F|iG \rangle, \quad (6)$$

so that for any (time-independent) hermitian F in $\mathcal{L}(\mathcal{H})$ the corresponding mean-value state functional can be written as $\langle F \rangle = \text{Tr}(\rho F) = \text{Tr}(\sqrt{\rho} F \sqrt{\rho}) = \langle \sqrt{\rho}|F|\sqrt{\rho} \rangle$, and can therefore be viewed as a functional of $\sqrt{\rho}$, the square-root density operator, obtained from the spectral expansion of ρ by substituting its eigenvalues with their positive square roots. When

... BUT IF ASSUMED AS A GENERAL FUNDAMENTAL DYNAMICAL PRINCIPLE (MAXIMAL ENTROPY GENERATION) IT CAN ALSO PROVIDE AN INTRIGUING, CONSISTENT, MICROSCOPIC-LEVEL UNIFICATION OF MECHANICS AND THERMODYNAMICS

5 MIT school unified theory of mechanics and thermodynamics

The growing interest during the last several decades in quantum dynamical models of systems undergoing irreversible processes has been motivated by impressive technological advances in the manipulation of smaller and smaller systems, from the micrometer scale to the nanometer scale, and down to the single atom scale. The laws of thermodynamics, that fifty years ago were invariably understood as pertaining only to macroscopic phenomena (an opinion still maintained by physicists of that generation, including several still active and influent members of the physical community), have gradually earned more attention and a central role in studies of mesoscopic phenomena first, and of microscopic phenomena more recently.

For a variety of ad-hoc reasons – statistical, phenomenological, information-theoretic, quantum-theoretic, conceptual – many investigators have concluded that the von Neumann equation of motion (Equation 2 with $\Delta M = 0$ identically) is incomplete, and a number of modification have been attempted [29].

During the last decades, though with very different interpretations and approaches, there has been a gradual convergence toward a new important innovation: the idea that entropy is a microscopic quantity and that irreversibility should be incorporated in the microscopic description (see e.g., [5]). The differences of interpretation and the various schools of thought still make this subject very controversial. But there is no doubt that credit for this fundamental ansatz, as well as for including it in a coherent and complete new quantum theory that goes beyond quantum mechanics without contradicting it, by incorporating equilibrium and nonequilibrium thermodynamics, must be given to the pioneering contributions of the MIT school [8, 3, 13, 14, 15, 30].

The implementation proposed by the MIT school provides an alternative to the traditional interpretation and the Information Theory interpretation of the successful mathematical formalism of Statistical Mechanics (SM). It retains all the successful aspects of its formalism within a sound conceptual framework free of inconsistencies and drastic departures from the traditional structure of a physical theory, in particular, with no need to abandon such keystones of traditional physical thought as the concept of trajectory and the principle of causality.

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, has been first proposed (without a dynamical law) by Hatsopoulos and Gyftopoulos [8] on physical and theoretical reasoning only (for a recent summary see [31]).

Thirty years ago, the hypothesis of a state domain aug-

ρ evolves according to Eq. (1), the rate of change of $\text{Tr}(\rho F)$ can be written as

$$d\text{Tr}(\rho F)/dt = \text{Tr}(F d\rho/dt) = 2 \langle \sqrt{\rho}|F|\sqrt{\rho}E(\rho) \rangle. \quad (7)$$

In particular, for the evolution equation to be well defined, the functional $\text{Tr}(\rho I)$ where I is the identity on \mathcal{H} must remain equal to unity at all times; therefore, $d\text{Tr}(\rho I)/dt = 2 \langle \sqrt{\rho}|I|\sqrt{\rho}E(\rho) \rangle = 0$, in view of Eq. (2) (implies the condition

$$\langle \sqrt{\rho}|\sqrt{\rho}\Delta M(\rho) \rangle = 0. \quad (8)$$

For F and G hermitian in $\mathcal{L}(\mathcal{H})$, we introduce the following shorthand notation

$$\Delta F = F - \text{Tr}(\rho F)I, \quad (9)$$

$$\langle \Delta F|\Delta G \rangle = \langle \sqrt{\rho}\Delta F|\sqrt{\rho}\Delta G \rangle = \frac{1}{2}\text{Tr}(\rho\langle \Delta F, \Delta G \rangle), \quad (10)$$

$$\Delta F = \sqrt{\sigma_{FF}} = \sqrt{\langle \Delta F|\Delta F \rangle}, \quad (11)$$

$$\begin{aligned} \langle (F, G)/2i \rangle &= \langle \sqrt{\rho}\Delta F|\sqrt{\rho}\Delta G \rangle = \frac{1}{2i}\text{Tr}(\rho\langle F, G \rangle) \\ &= \langle (F, G)/2i \rangle^* = -\langle (G, F)/2i \rangle, \end{aligned} \quad (12)$$

For example, we may write the rate of change of the mean value of a time-independent observable F as

$$\frac{d\text{Tr}(\rho F)}{dt} = \frac{\langle (F, H)/2i \rangle}{\hbar/2} + \frac{\langle \Delta F|\Delta M \rangle}{k_B\tau}, \quad (13)$$

from which we see that not all operators F that commute with H correspond to constants of the motion, but only those for which $\langle \Delta F|\Delta M \rangle = 0$, i.e., such that $\sqrt{\rho}\Delta F$ is orthogonal to both $i\sqrt{\rho}\Delta H$ and $\sqrt{\rho}\Delta M$, in the sense of scalar product (5). For an isolated system, conservation of the mean energy functional $\text{Tr}(\rho H)$ requires an operator function $\Delta M(\rho)$ that maintains $\sqrt{\rho}\Delta M$ always orthogonal to $\sqrt{\rho}\Delta H$, so that $\langle \Delta H|\Delta M \rangle = 0$ for every ρ .

We now consider the entropy functional $S = \text{Tr}(\rho S) = -k_B \text{Tr}(\rho \ln \rho) = -k_B \langle \sqrt{\rho}|\sqrt{\rho} \ln(\sqrt{\rho})^2 \rangle$ and its rate of change, which using Eqs. (2) and (8) may be written as

$$d\text{Tr}(\rho S)/dt = 2 \langle \sqrt{\rho}S|\sqrt{\rho}E(\rho) \rangle = \langle \Delta S|\Delta M \rangle / k_B\tau \quad (14)$$

where, for convenience, we define the entropy operator

$$S = -k_B P_{\rho>0} \ln \rho, \quad (15)$$

where $P_{\rho>0}$ is the projection operator onto the range of ρ [22]. Interestingly, the rate of entropy change, being proportional to the correlation coefficient between entropy measurements and M measurements, under the assumptions made so far, may be positive or negative, depending on how M is defined, i.e., depending on the specifics of the physical model in which Eq. (2) is adopted.

3 Steepest-entropy-ascent, conservative dissipative dynamics of an isolated system

We now further assume the explicit form of $\Delta M(\rho)$ that yields steepest-entropy-ascent, conservative dissipative dynamics [12, 17, 18, 19]

$$\Delta M(\rho) = \Delta S - \Delta H'(\rho)/\theta(\rho), \quad (16)$$

where S is the entropy operator defined in (15),

$$\Delta H'(\rho) = \Delta H - \mu(\rho) \cdot \Delta \mathbf{N}, \quad (17)$$

H is the Hamiltonian, $\mathbf{N} = \{N_1, \dots, N_r\}$ (a possibly empty set of operators commuting with H , that we call non-Hamiltonian generators of the motion (for example, the number-of-particles operators or a subset of them, or the momentum component operators for a free particle), such that operators $\sqrt{\rho}\Delta H$ and $\sqrt{\rho}\Delta \mathbf{N}$ are linearly independent, $\theta(\rho)$ and $\mu(\rho) = \{\mu_1(\rho), \dots, \mu_r(\rho)\}$ a set of real functionals defined for each ρ by the solution of the following system of linear equations

$$\langle \Delta S \Delta H \rangle \theta + \sum_{i=1}^r \langle \Delta N_i \Delta H \rangle \mu_i = \langle \Delta H \Delta H \rangle, \quad (18)$$

$$\langle \Delta S \Delta N_j \rangle \theta + \sum_{i=1}^r \langle \Delta N_i \Delta N_j \rangle \mu_i = \langle \Delta H \Delta N_j \rangle, \quad (19)$$

which warrant the conditions that $\langle \Delta H \Delta M \rangle = 0$ and $\langle \Delta N_j \Delta M \rangle = 0$, and hence that the mean values $\text{Tr}(\rho H)$ and $\text{Tr}(\rho \mathbf{N})$ are maintained time invariant by the dissipative term of the equation of the motion.

Operators $\sqrt{\rho}\Delta H'$ and $\sqrt{\rho}\Delta M$ are always orthogonal, in the sense that $\langle \Delta M \Delta H' \rangle = 0$ for every ρ . It follows that, in general, $\langle \Delta S \Delta H' \rangle = \langle \Delta H' \Delta H' \rangle / \theta$,

$$\langle \Delta S \Delta M \rangle = \langle \Delta M \Delta M \rangle = \langle \Delta S \Delta S \rangle - \frac{\langle \Delta H' \Delta H' \rangle}{\theta^2(\rho)} \geq 0, \quad (20)$$

and hence the rate of entropy generation (14) is always strictly positive except for $\langle \Delta M \Delta M \rangle = 0$ (which occurs iff $\sqrt{\rho}\Delta M = 0$), i.e., for $\sqrt{\rho_{\text{nd}}}\Delta S_{\text{nd}} = \langle \sqrt{\rho_{\text{nd}}}\Delta H - \mu_{\text{nd}} \cdot \sqrt{\rho_{\text{nd}}}\Delta \mathbf{N} \rangle / \theta_{\text{nd}}$, for some real scalars θ_{nd} and μ_{nd} , that is, for density operators (that we call non-dissipative) of the form

$$\rho_{\text{nd}} = \frac{B \exp[-(H - \mu_{\text{nd}} \cdot \mathbf{N})/k_B\theta_{\text{nd}}]B}{\text{Tr}B \exp[-(H - \mu_{\text{nd}} \cdot \mathbf{N})/k_B\theta_{\text{nd}}]}, \quad (21)$$

where B is any projection operator on \mathcal{H} ($B^2 = B$).

The nonlinear functional $\theta(\rho) = \langle \Delta H' \Delta H' \rangle / \langle \Delta S \Delta H' \rangle$ may be interpreted in this framework as a natural generalization to nonequilibrium of the temperature, at least insofar as for $t \rightarrow +\infty$, while the state operator $\rho(t)$ approaches a non-dissipative operator of form (21), $\theta(t)$ approaches smoothly the corresponding thermodynamic equilibrium (or partial equilibrium) temperature θ_{nd} .

mented with respect to that of traditional QM was perceived as adventurous [32] and countercurrent to the prevailing approaches to dissipative quantum dynamics within the frameworks of statistical, stochastic, phenomenological, information-theoretic, chaotic-behavior and bifurcation theories.

The recent new experimental evidence of loss of quantum coherence [9, 33, 34] and the impressive effort devoted to study nonlinear modifications of the standard Schrödinger equation in the last twenty years [35], finally seem to make more acceptable, if not require, the $\rho^2 \neq \rho$ augmented state domain Hatsopoulos–Gyftopoulos (HG) ansatz.

Once the $\rho^2 \neq \rho$ ansatz is accepted, the nonlinear equation of motion we proposed completes the dynamics and holds the promise to provide a microscopic-level explanation of the recent experimental evidence of loss of quantum coherence. It is with this motivation that Gheorghiu-Svirschchevski [5, 2] has ‘rediscovered’ our Equation (2) together with many of its known features, including existence and uniqueness of solutions, an elegant and useful expansion, and other results in the near-equilibrium linear limit. However, in Ref. [5] the question of defining the form of the relaxation-time functional is left unresolved, together with the nontrivial problem to extend the nonlinear dynamics to composite systems with internal partitions between separated subsystems, that we address in [15, 17].

The fact that nonidempotent density operators ($\rho^2 \neq \rho$) are considered also in SM and are referred to as mixed states may generate some confusion and requires an important clarification. In SM, mixed states are used to represent heterogeneous preparations, and the functional $-\text{Tr}(\rho \ln \rho)$ as a statistical indicator of the heterogeneity of a preparation. Instead, the essence of the HG ansatz is the observation that in general we need nonidempotent density operators to represent unambiguously homogeneous preparations.

A preparation is homogeneous if it generates an ensemble of identical systems which cannot be conceivably subdivided into subensembles different from the original ensemble. Notice that for two ensembles of identical systems to be different it suffices that the arithmetic mean value of data yielded by measurements of a physical observable on the member systems of one of the two ensembles be different from the mean value of data yielded by measurements of the same physical observable on the member systems of the other ensemble.

Since, by definition, there exist no subdivisions of a homogeneous ensemble into different subensembles, it follows that each individual member system of a homogeneous ensemble has exactly the same intrinsic characteristics as any other member. For, if all member systems did not have the same intrinsic characteristics, then it would be possible to conceive of subdivisions of the ensemble into subensembles that are not identical.

The whole of these intrinsic characteristics, shared by all the

Because here H always commutes with M , $c_{MH} = 0$ and $\langle M|i\dot{H} \rangle = 0$, which means that $\sqrt{\rho}\Delta M(\rho)$ is always orthogonal to $i\sqrt{\rho}\Delta H$. This reflects the fact that on the entropy surface the direction of steepest entropy ascent is orthogonal to the (constant entropy) orbits that characterize purely Hamiltonian (unitary) motion (in which the entropy is maintained constant by keeping invariant each eigenvalue of ρ).

As shown in Refs. [13], the dissipative dynamics generated by Eq. (2) with $\Delta M(\rho)$ as just defined and a time-independent Hamiltonian H : (i) maintains $\rho(t) \geq \rho^2(t)$ at all times, both forward and backward in time for any initial density operator $\rho(0)$ (see also [5, 17]); (ii) maintains the cardinality of $\rho(t)$ invariant; (iii) entails that the entropy functional is an S -function in the sense defined in [21] and therefore that maximal entropy density operators obtained from (21) with $B = I$ are the only equilibrium states of the dynamics that are stable with respect to perturbations that do not alter the mean values of the energy and the other time invariants (if any): this theorem of the dynamics coincides with a well-known general statement of the second law of thermodynamics [8, 23]; (iv) entails Onsager reciprocity in the sense defined in [16]; (v) can be derived from a variational principle [5, 17], equivalent to our steepest entropy ascent geometrical construction [13, 19], by maximizing the entropy generation rate subject to the $\text{Tr}(\rho)$, $\text{Tr}(\rho H)$, and $\text{Tr}(\rho \mathbf{N})$ conservation constraints and the additional constraint $\langle \sqrt{\rho}E|\sqrt{\rho}E \rangle = c(\rho)$ [17, 19].

We finally note that assuming in Eq. (2), in addition to $\Delta M(\rho)$ given by (16), the nonlinear relaxation time $\tau(\rho)$ given by [17, 19]

$$\tau(\rho) = \hbar \Delta M / 2k_B \Delta H, \quad (22)$$

we obtain the most dissipative (maximal entropy generation rate [17]) dynamics in which the entropic characteristic time [19] $\tau_S = \Delta S / d\langle S \rangle / dt$ is always compatible with the time-energy uncertainty relation $\tau_S \Delta H \geq \hbar/2$ and the rate of entropy generation is always given by $2\Delta M \Delta H / \hbar$.

The usefulness and physical meaning of the proposed nonlinear model equation is worth further investigations and experimental validation in specific far nonequilibrium contexts in which linear models of Lindblad form are insufficient. One such context may be the currently debated so-called ‘fluctuation theorems’ [24] whereby fluctuations and, hence, uncertainties are measured on a microscopic system (optically trapped colloidal particle [25], electrical resistor [26]) driven at steady state (off thermodynamic equilibrium) by means of a work interaction, while a heat interaction (with a bath) removes the entropy being generated by irreversibility. Another such context may be that of pion-nucleus scattering, where available experimental data have recently allowed partial validation [27] of ‘entropic’ uncertainty relations [28]. Yet another is within the model we propose in Ref. [18] for the description of the irreversible time evolution of a perturbed, isolated, physical system during relaxation toward thermodynamic equilibrium by spontaneous internal rearrangement of the occupation probabilities. We pursue this example in the next section.

4 Numerical example

To illustrate the well behaved time dependence implied by the proposed dynamical law, we consider an isolated, closed system composed of noninteracting identical particles with single-particle eigenstates with energies ϵ_i for $i = 1, 2, \dots, N$, where N is assumed finite for simplicity and the ϵ_i 's are repeated in case of degeneracy, and we restrict our attention to the class of dilute-Boltzmann-gas states in which the particles are independently distributed among the N (possibly degenerate) one-particle energy eigenstates. This model is introduced in Ref. [18], where for our generalized nonequilibrium Massieu-function operator we assume the form

$$M(\rho) = S - H/\theta(\rho), \quad (23)$$

and, therefore,

$$\Delta M(\rho) = \Delta S - \Delta H/\theta(\rho). \quad (24)$$

For simplicity and illustrative purposes, we focus on purely dissipative dynamics by considering a particular trajectory $\rho(t)$ that commutes with H at all times t , assuming that H is time independent and has a nondegenerate spectrum. As a result, the energy-level occupation probabilities p_n coincide with the eigenvalues of ρ , and the dynamical equation reduces to the simple form [18]

$$\frac{dp_n}{dt} = -\frac{1}{\tau} \left[p_n \ln p_n + p_n \frac{\langle S \rangle}{k_B} + p_n e_n - \langle H \rangle \right], \quad (25)$$

where

$$\langle S \rangle = -k_B \sum_n p_n \ln p_n, \quad (26)$$

$$\langle H \rangle = \sum_n p_n e_n, \quad (27)$$

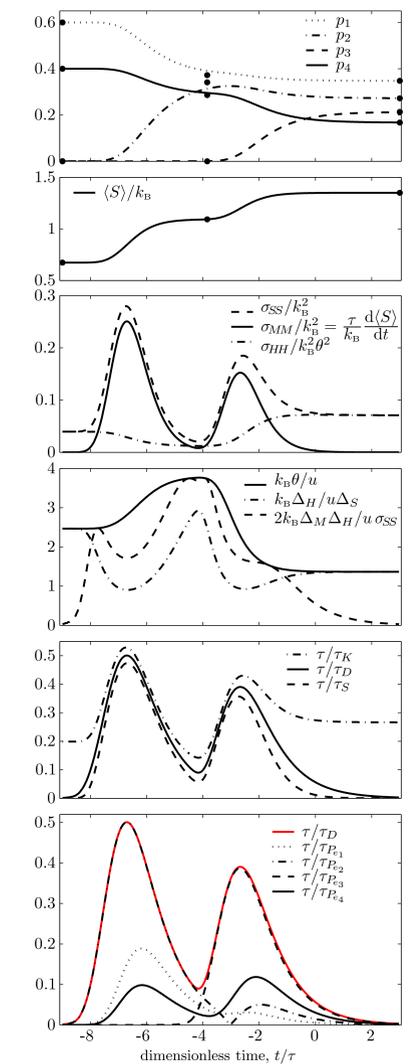
$$\theta = \frac{\langle \Delta H \Delta H \rangle}{\langle \Delta H \Delta S \rangle}, \quad (28)$$

$$\langle \Delta H \Delta H \rangle = \sum_n p_n e_n^2 - \langle H \rangle^2, \quad (29)$$

$$\langle \Delta H \Delta S \rangle = -k_B \sum_n p_n e_n \ln p_n - \langle H \rangle \langle S \rangle. \quad (30)$$

The plots in Figure 1, illustrate a sample trajectory obtained by solving numerically, both forward and backward in time, the system of nonlinear equations (25) for an initial state with cardinality equal to 4 and τ assumed constant, with nonzero occupation probabilities only for the four energy levels $\epsilon_1 = 0$, $\epsilon_2 = u/3$, $\epsilon_3 = u/3$, and $\epsilon_4 = u$, and with mean energy $\langle H \rangle = 2u/5$ (u is arbitrary, with units of energy). As done in [18], the initial state $\rho(0)$ at time $t = 0$ is selected so that the

resulting trajectory $\rho(t)$ passes in the neighborhood of the partially canonical nondissipative state $\rho_{\text{nd}}^{\text{pc}}$ that has nonzero occupation probabilities only for the three energy levels ϵ_1 , ϵ_2 , and ϵ_4 , and mean energy $\langle H \rangle = 2u/5$ ($\rho_{\text{nd}}^{\text{pc}} = 0.3725$, $\rho_{\text{nd}}^{\text{pc}} = 0.3412$, $\rho_{\text{nd}}^{\text{pc}} = 0$, $\rho_{\text{nd}}^{\text{pc}} = 0.2863$, $\theta_{\text{nd}}^{\text{pc}} = 3.796 u/k_B$). During the first part of the trajectory, this nondissipative state appears as an attractor, an approximate or ‘false target’ equilibrium state; when the trajectory gets close to this state, the evolution slows down, the entropy generation drops almost to zero and the value of θ gets very close ($3.767 u/k_B$) to that of $\theta_{\text{nd}}^{\text{pc}}$; however eventually the small, but nonzero initial occupation of level ϵ_3 builds up and a new rapid rearrangement of the occupation probabilities takes place, and finally drives the system toward the maximal entropy state $\rho_{\text{nd}}^{\text{pc}}$ with energy $\langle H \rangle = 2u/5$ and all four active levels occupied, with partially canonical distribution $\rho_{\text{nd}}^{\text{pc}} = 0.3474$, $\rho_{\text{nd}}^{\text{pc}} = 0.2722$, $\rho_{\text{nd}}^{\text{pc}} = 0.2133$, $\rho_{\text{nd}}^{\text{pc}} = 0.1671$, and characterized according to (21) by the (partial equilibrium) temperature $\theta_{\text{nd}}^{\text{pc}} = 1.366 u/k_B$.



The top subfigure shows the four nonzero occupation probabilities as functions of dimensionless time: t/τ . The dots on the right represent the maximal entropy distribution, $p_n(+\infty) = p_n^{\text{pc}}$; the dots at the left represent the lowest-entropy or ‘primordial’ distribution, $p_n(-\infty) = p_n^{\text{nd}}$, which for the particular trajectory selected here, corresponds to a nondissipative state $\rho_{\text{nd}}^{\text{nd}}$ that has only two occupied energy levels, ϵ_1 and ϵ_4 , with probabilities $p_{\text{nd}}^{\text{nd}} = 0.6$ and $p_{\text{nd}}^{\text{nd}} = 0.4$ (and temperature $\rho_{\text{nd}}^{\text{nd}} = 2.466 u/k_B$); in fact the system has no lower entropy states ρ that commute with H , have energy $2u/5$, and have zero occupation probabilities p_n for every $n > 4$ [18]. The dots in the middle represent the nondissipative state $\rho_{\text{nd}}^{\text{pc}}$ which appears as the false target state during the first part of the trajectory, plotted at the instant in time when the entropy of the time-varying trajectory is equal to the entropy of this distribution.

The second subfigure shows the time dependence of the dimensionless entropy $\langle S \rangle / k_B$; the third shows its rate of change (proportional to $\langle \Delta M \Delta M \rangle$) and compares it with $\langle \Delta S \Delta S \rangle$ and $\langle \Delta H \Delta H \rangle / \theta^2$; the fourth shows the time dependence of our generalized ‘nonequilibrium temperature’ θ (properly nondimensionalized) and compares it with $\Delta H / \Delta S$ and $2\Delta M \Delta H / \sigma_{SS}$ where $\sigma_{SS} = \langle \Delta S \Delta S \rangle$; the fifth subfigure shows the time dependence of $1/\tau_{TD}$ (which here is proportional to the square root of the rate of entropy generation, third subfigure) and compares it with $1/\tau_K$ and $1/\tau_S$, where [19] $\tau_{TD} = k_B\tau/\Delta M$, $\tau_K = k_B\tau/\Delta S$; the sixth subfigure shows $1/\tau_{PC}$ for each of the four occupation probabilities and compares them with $1/\tau_{TD}$, where [19] $\tau_{PC} = \sqrt{\langle \Delta P_{\epsilon_i} \Delta P_{\epsilon_i} \rangle} / (dp_n/dt)$.

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