Information compressibility, entropy production and approach to steady state in open systems

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We introduce the concept of information compressibility, $K_I$, which measures the relative change of number of available microstates of an open system in response to an energy variation. We then prove that at the time in which the system reaches a steady state, the second and third time derivatives of the information entropy are proportional to the corresponding time derivatives of the energy, the proportionality constant being $K_I$. We argue that if two steady states with different but same-sign $K_I$ are dynamically connected in a non-adiabatic way it takes a longer time to reach the state with compressibility closer to zero than the reverse. This concept, that applies to both classical and quantum open systems, thus provides insight into the properties of non-equilibrium steady states.

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Dynamical systems are to some extent always in interaction with one or more external environments. The latter ones may exchange particles and/or energy with the system of interest. Under certain conditions this leads to a non-equilibrium steady state (NESS) of the system dynamics. This situation arises in various physical systems, from chemical and biological processes to nanoscale systems. The properties of NESSs, whether quantum or classical, have long been the subject of numerous studies but a comprehensive theoretical description is still lacking, especially for NESSs far from equilibrium. One aspect, in particular, that has received much less attention is the approach to steady state, and the entropy production in such instance.

The difficulty in describing properties of NESSs and the approach to steady state can be in part attributed to the lack of a general physical quantity that characterizes such states, especially far from thermodynamic equilibrium. Such a quantity needs to take into account the microscopic dynamics of the system and, at the same time, provide a global physical description that is, in principle, easy to access theoretically and/or experimentally.

In this Letter we introduce such a quantity that we name information compressibility, $K_I$. The latter measures the “easiness,” or “difficulty,” to vary the relative number of available microstates of an open system when its energy changes due to the interaction with the environment(s). This concept is the information counterpart of the similar concept for solids, liquids or gases, where the standard compressibility quantifies the relative change of the volume with respect to a pressure variation.

The advantage of the information compressibility in characterizing non-equilibrium systems stems from the fact that it allows us to establish several results regarding the approach to steady state. In fact, we prove analytically that at the time in which the system reaches a steady state the second and third time derivatives of the information entropy are proportional to the corresponding time derivatives of the energy. In both cases, the proportionality constant is $K_I$ at that instant of time. The entropy production at that moment can be thus minimal or maximal according to the sign of the information compressibility and the concavity or convexity of the energy function. In addition, we can argue about the time it takes the system to reach a steady state with a given information compressibility from another steady state with different $K_I$, when the two are connected non-adiabatically. We find that when the two compressibilities have the same sign it takes a longer time to reach the state with compressibility closer to zero than the reverse process. The reason for this behavior can be intuitively attributed to the fact that the fluctuations induced by the presence of the environment act against the first process, while they “help” the second one. No such conclusion can be reached if the two states have compressibilities of different sign. Therefore, this concept, that applies to both quantum and classical open systems, provides insight into the properties of non-equilibrium steady states. We will illustrate these findings with a model of a two-level system in contact with two thermal baths.

Definition of information compressibility— By varying the energy of an open system the number of microstates (in the appropriate phase space) available to it generally changes. This means that there is a loss – or gain – of information when the system interacts with the environment(s). By energy and entropy we mean the following.

Consider the many-body Hamiltonian

$$\hat{H}_{tot} = \hat{H}_S + \hat{H}_B + \hat{H}_{int}, \quad (1)$$

where $\hat{H}_S$ is the Hamiltonian of the system we are interested in, $\hat{H}_B$ is the Hamiltonian of the bath(s) degrees of freedom, and $\hat{H}_{int}$ describes their mutual interaction. The above Hamiltonians may describe either a quantum or a classical system. To be specific, from now on we refer to the quantum case only, but all considerations we
make apply also to the classical case, with the appropriate change of quantities (e.g., the replacement of the density matrix \( \hat{\rho} \) with the classical phase density).

Call \( \hat{\rho}_{\text{tot}} \) the density matrix associated with the total Hamiltonian. We may then define the reduced density matrix \( \hat{\rho} \) of the system alone by tracing out the degrees of freedom of the bath(s), namely

\[
\hat{\rho} = \text{Tr}_B\{\hat{\rho}_{\text{tot}}\}.
\] (2)

Note that, in general, there is no closed equation of motion for \( \hat{\rho} \). At this stage, this is of no concern to us and we assume that we know this operator at any given time. We can then define the average energy of the system as

\[
E(t) = \text{Tr}\{\hat{\rho}(t)\hat{H}_S\},
\] (3)

and the information entropy

\[
S(t) = -k_B\text{Tr}\{\hat{\rho}(t) \ln \hat{\rho}(t)\},
\] (4)

with \( k_B \) the Boltzmann’s constant.

Call \( \Omega \) the number of microstates available to the system at any given time. In analogy with the standard compressibility of matter we can thus define the information compressibility as

\[
K_I(t) = \frac{1}{k_B} \frac{\delta \Omega}{\delta E}\bigg|_{E(t)},
\] (5)

namely the relative variation of the number of microstates with respect to an energy variation, evaluated at the instantaneous energy.

This definition, however, would require an explicit calculation of the number of available microstates. This is not always easy to do. We thus seek an equivalent definition that is computationally more convenient. We note first that in micro-canonical equilibrium the number of available microstates is related to the entropy \( S \) of the system via the relation \( \Omega = \exp(S/k_B) \). If we introduce such definition into Eq. (5) we get

\[
K_I(t) = \frac{1}{k_B} \frac{\delta S}{\delta E}\bigg|_{E(t)}. \tag{6}
\]

We could choose Eq. (6) as definition of information compressibility in the general case as well, with the information entropy given by Eq. (4). Note that despite its similarity with the well-known equilibrium quantity \( \beta = 1/k_BT \), with \( T \) the temperature, Eq. (6) depends on time, and therefore it cannot be generally interpreted as an inverse thermal energy (except at canonical equilibrium, see discussion below). In addition, the functional dependence of the entropy on the energy is not always known and definition (6) is thus of limited use, except for specific cases. Instead, both the information entropy and the energy are generally accessible at any given time, which implies that their time derivatives are known functions. We thus replace the definition (6) with the following — computationally more convenient — form

\[
K_I(t) \equiv \frac{1}{k_B} \frac{\partial S}{\partial E} \frac{\partial E'}{\partial t'}\bigg|_{t'=t},
\] (7)

with \( S(t) \) and \( E(t) \) evaluated as in Eqs. (4) and (3), respectively. This is the definition of information compressibility we postulate from now on.

Before discussing the open-system problem let us check the physical meaning of Eq. (7) for known cases. First of all, we realize that if the system is in a steady state the energy variation is zero, as well as the entropy variation. The information compressibility would thus acquire a constant value, with such constant dependent on the dynamics of the system approaching the given steady state. In addition, the information compressibility (7) may be either positive or negative at any given time, with the negative sign indicating an increase (decrease) of entropy with decreasing (increasing) energy supplied to the system by the environment(s).

For a closed system the information entropy does not vary in time, irrespective of the energy variation \( \delta E \). Therefore, as expected, the information compressibility for closed systems is zero at any given time: no matter how much the energy of a closed system varies, the number of available microstates is constant in time (property of the unitary evolution).

Let us now consider a system in global canonical equilibrium with a bath at temperature \( T \). In this case the entropy is

\[
S_C = k_B \ln Z_C + E_{eq}/T,
\]

where \( E_{eq} = \text{Tr}\{\hat{\rho}_{eq}^{\text{tot}}\hat{H}_S\} \) is the average energy of the system at equilibrium, \( Z_C \) is the canonical partition function, and \( \hat{\rho}_{eq}^{\text{tot}} \) the canonical density matrix. By differentiating this entropy with respect to the energy (at fixed volume and number of particles) we get

\[
K_I^C = 1/k_BT,
\]

which is the well-known quantity \( \beta \) of equilibrium statistical mechanics. The information compressibility is thus a natural extension of \( \beta \) to the non-equilibrium case, where the concept of temperature is ill-defined.

This result also shows that the higher the temperature the more difficult it is to change the relative volume of available microstates. In fact, a large temperature means a highly-disordered state, and it is thus natural to think that, for a given small energy variation, the relative change of entropy (or level of disorder) would be small by adding (or subtracting) more states. Conversely, a small temperature means more order in the system. A small change in energy thus produces a relatively larger change in the number of microstates available to the system.

**Approach to steady state**— To illustrate the usefulness of the concept of information compressibility, let us now examine the role of \( K_I \) in the approach to steady state.
If we differentiate Eq. (7) with respect to time we get
\[ k_B \frac{dK_i}{dt} \frac{dE}{dt} = \frac{d^2S}{dt^2} - k_B K_i \frac{d^2E}{dt^2}. \] (8)

Let us now assume that the system reaches a steady state during time evolution. Call \( t_{ss} \) the time at which this occurs. At steady state \( dK_i/dt = 0 \) (as well as \( dE/dt = 0 \)) so that from Eq. (8) we get
\[ \frac{d^2S}{dt^2} \bigg|_{t=t_{ss}} = k_B K_i \frac{d^2E}{dt^2} \bigg|_{t=t_{ss}}, \] (9)
where \( t = t_{ss} \) means the limit in which the time approaches \( t_{ss} \) from the past. The above relation shows that the entropy production (i.e., the time variation of the entropy) can be either maximal or minimal at the onset of steady state. This depends on both the concavity or convexity of the energy function – i.e., whether the energy is supplied to or taken away from the system by the environment(s) – and the sign of the information compressibility. Note also that the reverse is not necessarily true: the validity of Eq. (9) is not sufficient to guarantee that the system is in a steady state.

We can differentiate once more Eq. (8), and at steady state we obtain the relation
\[ \frac{d^3S}{dt^3} \bigg|_{t=t_{ss}} = k_B K_i \frac{d^3E}{dt^3} \bigg|_{t=t_{ss}}, \] (10)
which is an even stronger property than Eq. (9). However, further differentiation of Eq. (5) does not provide a simple relation between the \( n \)-th time derivative of the entropy and the \( n \)-th time derivative of the energy, even at steady state. The reason is that time derivatives of \( K_i \) of order higher than one appear in such expression, and these derivatives are not necessarily zero at \( t_{ss} \).

Having discussed the entropy production at steady state, let us now apply the above concept to study the time it takes the system to go from a given steady state with information compressibility, \( K_i^{(1)} \), to a steady state with different (but equal sign) compressibility, \( K_i^{(2)} \), and the reverse process (see inset of Fig. 1). Let us call \( S_1 \) and \( E_1 \), the information entropy and the energy of the first steady state, respectively, and \( S_2 \) and \( E_2 \), the corresponding quantities of the second.

We are concerned here with two different steady states which are connected non-adiabatically, and have the same-sign \( K_i \). For clarity, let us assume
\[ K_i^{(1)} > K_i^{(2)}, \] (11)
and both quantities are positive. Let us first consider the time \( t_{ss}^{(1)} \) at which we increase the energy of the system (which implies that the entropy increases as well) so that the latter evolves from the steady state 1 to the steady state 2 (\( dK_i/dt < 0 \)). Referring to Eq. (8), we then see that its lhs is a negative quantity. Since, by assumption, both \( d^2S_1/dt^2 \) and \( d^2E_2/dt^2 \) are positive at \( t_{ss}^{(1)} \), we find that at that instant
\[ \frac{d^2S_1}{dt^2} < k_B K_i^{(1)} \frac{d^2E_1}{dt^2}, \] (12)
namely the entropy variation is “slower” than the corresponding energy variation. If we repeat the same reasoning for the time \( t_{ss}^{(2)} \) at which we reduce the energy (and entropy) to recover steady state 1 from steady state 2, [9] we find instead
\[ \frac{d^2S_2}{dt^2} > k_B K_i^{(2)} \frac{d^2E_2}{dt^2}, \] (13)
namely the disorder varies faster than the corresponding energy variation. We thus argue that it takes longer to reach the steady state with compressibility closer to zero than the reverse process. The same can be concluded for two steady states with negative compressibilities. This reflects the intuitive notion that the fluctuations induced by the presence of the environment act against the “compression” of the volume of available microstates, while they favor the reverse process.

Note that one cannot say anything about the time scales when the compressibilities of the two steady states differ in sign. In such a case, applying the above argument leads to the obvious mathematical statement that a negative number is smaller than a positive one, thus precluding any conclusion on the time scales of the two processes.

**Example** — We conclude by illustrating the above results for a specific model system. We study a quantum two-level system in contact with two heat baths kept at two different temperatures. We work in the Markovian approximation and use the Lindblad equation (\( \hbar = 1 \)) [10, 11],
\[ \dot{\rho} = -i[\mathcal{H}, \rho] + \mathcal{L}_1 \rho + \mathcal{L}_2 \rho, \] (14)

\[ \mathcal{L}_i = -\frac{1}{2}(V_i^\dagger V_i, \rho) + V_i \rho V_i^\dagger, \quad i = 1, 2 \]
where \( \rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{12}^\dagger & 1 - \rho_{11} \end{pmatrix} \) is the density matrix, and the Hamiltonian and relaxation operators are given by [11]
\[ \mathcal{H} = \begin{pmatrix} \omega & 0 \\ 0 & 0 \end{pmatrix}, \quad V_i = \gamma_i^{1/2} \begin{pmatrix} 0 \\ \exp\left(-\frac{\omega}{4k_B T_i}\right) \end{pmatrix}, \quad V_i^\dagger = \gamma_i^{1/2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \] (15)
Here \( T_i \) \((i = 1, 2)\) is the temperature of the \( i \)-th bath, \( \omega \) is the two-level energy separation, and \( \gamma_i = \gamma_0 \cosh \left(\frac{\omega}{2k_B T_i}\right) \) is a normalization factor with \( \gamma_0 \) some relaxation rate. This form is chosen such that detailed balance is satisfied for each thermal bath independently,
The analytical solution of Eq. (13) for arbitrary times is too cumbersome to be presented here. We thus show only the main results. We have calculated the dynamics of the system as it approaches a steady state, and validated our results with a simple example of a two-level system in contact with two heat baths. The concepts and results described here are, in principle, testable within present experimental model systems and we hope this work will motivate studies in this direction.

Finally, we believe that the concept of information compressibility can be a valuable tool in studying the dynamics of out-of-equilibrium phenomena, and may be useful in characterizing, for instance, dynamical phase transitions such as the glass transition, where the system’s properties vary dramatically.

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5 In fact, since the entropy is a non-linear functional of the density matrix, while the energy is a linear one, Eq. (6) may even provide multiple values at specific times.
7 Note that this time may be infinite.
8 An adiabatic path between the two steady states results, by construction, in a time-symmetric evolution from one to the other, and vice versa.
9 We are assuming here that all these times are finite.
12 One can, in fact, choose different normalizations for the Lindblad operators. Such a change does not affect the re-
results presented here qualitatively.