ON COARSE-GRAINED ENTROPY AND MIXING IN STATISTICAL MECHANICS

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ABSTRACT. The object of the paper is the study of the roles of non-equilibrium entropy and mixing of phases in the statistical characterization of the coarse-grained interpretation of the irreversible approach to statistical equilibrium of an isolated system.

KEY WORDS AND PHRASES. Probability space, σ -algebra, observational states, sufficient partition, Coarse-grained distribution, Ergodicity, and Weak-mixing.

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1. INTRODUCTION.

The process of coarse-graining which is equivalent to the statistical averaging of the micro-states over the various phase-cells plays a significant role in the study of the macroscopic property of irreversibility from the reversibility of dynamical equations of motion. The coarse-graining cannot be done arbitrarily and Gibbs entropy based on an arbitrary coarse-grained distribution does not always ensure the relaxation to statistical equilibrium. The object of the present paper is to introduce a non-equilibrium entropy after Goldstein and Penrose [1] and to study the importance of ergodicity and mixing in the statistical characterization of the irreversible approach to statistical equilibrium of a classical isolated system.

2. DYNAMICAL SYSTEM AND OBSERVATIONAL STATES.

Let us consider a classical dynamical system whose dynamical state is given by (Ω, T_t) where Ω is the phase-space consisting of all possible phase-points and $\{T_t\}$ is the family of time-evolution transformations (automorphisms) defined for all real t generated by the dynamical equation of motion in phase-space Ω . Let m be the invariant Liouville's measure of phase-space and let ν be any other measure absolutely continuous to m . The probability density of microstates $\rho(\omega)$ is defined by a normalized density given by the Radon-Nikodym derivative

$$\rho(\omega) = \frac{d\nu}{dm}(\omega) \quad (2.1)$$

The time-evolution of the measure ν consists of the family of measures $\{\nu_t\}$ defined by [1]

$$\nu_t(T_t \omega) = \nu(\omega). \quad (2.2)$$

This implies that for any set $A \in \Omega$

$$\nu_t(A) = \nu(T_{-t} A). \quad (2.3)$$

The statistical structure (or model) of the system by the probability-space $(\Omega, A, \{\nu_t\})$ where A is the σ -algebra of subsets of Ω including itself, and, $\{\nu_t\}$ is the family of probability measures on A .

To determine the observational states of the system at the initial time $t = 0$ we divide the time of observation into a countably infinite number of intervals of equal length. Considering the length of each interval as the unit of the measurement of time, the evolution of a subset A in the course of time is given by the series $T_t A$ ($t = \dots, -2, -1, 0, 1, 2, \dots$). Let us define a partition P of phase-space into sets of points that are indistinguishable by an observation made at time $t = 0$. Two phase points ω_1 and ω_2 are then observationally equivalent if and only if the time translates $T_t \omega_1$ and $T_t \omega_2$ which lie, for every non-negative integer t , in the same set from the partition P . In other words, ω_1 and ω_2 must lie in the same set from the partition $T_t P$. Let us define the σ -algebra

$$\mathcal{A} = \bigvee_{t=0}^{\infty} T_{-t} P \quad (2.4)$$

as the smallest σ -algebra which contains all the partitions $P, T_{-1}P, T_{-2}P, \dots$. Thus every set in $\mathcal{A}$ is the image under of some set in $\mathcal{A}$; that is, to say, the σ -algebra $\mathcal{A}$ consists of image under T_t of all sets belonging to and includes (among others) all the sets of $\mathcal{A}$ itself [1]:

$$T_t \mathcal{A} \supset \mathcal{A} \quad (2.5)$$

The condition (2.5) is the condition of loss of observational information and represents the asymmetry between past and future [1].

3. NON-EQUILIBRIUM ENTROPY: IRREVERSIBILITY AND MIXING.

The entropy (fine-grained) of the classical dynamical system is defined by the functional

$$\begin{aligned} S(\nu_t, A) &= -K \int \rho_t(\omega) \log \rho_t(\omega) \, d\mu(\omega) \\ &= -k \int \log (d\nu_t/d\mu) \, d\nu_t(\omega). \end{aligned} \quad (3.1)$$

The entropy $S(\nu_t, A)$ defined over the fine grained-density $\rho_t(\omega)$ contains full information about the system. For observation behavior of the system such detailed information or description about the system is not necessary. For this a coarse-graining of microstates is necessary [2].

Let us consider the coarse-grained density $\bar{\rho}_t$ as the conditional expectation of $\rho_t(\omega)$ with respect to the σ -algebra $\mathcal{A}$ (which is the conditional expectation for the

measure $m/m(\mathcal{A})$ [1].

$$\bar{\rho}_t = E(\rho(\omega) | \mathcal{A}) \quad (3.2)$$

The entropy for the non-equilibrium state is then defined by the coarse-grained entropy [1]

$$\tilde{S}(v_t, \mathcal{A}) = -K \int \bar{\rho}_t \log \bar{\rho}_t \, dm(\omega). \quad (3.3)$$

Since the measure m used in defining the entropy is invariant, we have,

$$\tilde{S}(v_t, \mathcal{A}) = \tilde{S}(v, T_{-t}\mathcal{A}). \quad (3.4)$$

From (2.5), we have

$$T_{-t} \mathcal{A} \subset \mathcal{A}, \quad (t > 0). \quad (3.5)$$

As a consequence of (3.5), it is easy to prove that

$$\tilde{S}(v, T_{-t}\mathcal{A}) > \tilde{S}(v, \mathcal{A}) \quad (3.6)$$

or by (3.4), we have

$$\tilde{S}(v_t, \mathcal{A}) > \tilde{S}(v, \mathcal{A}), \quad (t > 0) \quad (3.7)$$

which proves the non-decreasing property of the entropy $\tilde{S}(v_t, \mathcal{A})$ with time; that is, the H-theorem.

The equality in (3.7) corresponds to the stationary state of statistical equilibrium of the system at the initial time $t = 0$. Mathematically this holds for the measure-preserving automorphism T_t :

$$v_t = v$$

or

$$vT_{-t} = v.$$

(3.8)

Also the equality in (3.6), which is a consequence of the relation (3.5), holds for the invariance relation:

$$T_{-t}\mathcal{A} = \mathcal{A}. \quad (3.9)$$

Thus the inequality in (3.7) for statistical equilibrium at the initial time $t = 0$ corresponds to the invariance of the σ -algebra $\mathcal{A}$ under measure-preserving automorphism T_t that is, to the condition of ergodicity of the system. The equality has also an important statistical significance. This, in fact corresponds to the sufficiency of the σ -algebra $\mathcal{A}$ or to the sufficient partitioning of microstates (or phase-space) into equivalent class of macrostates of the system [3.4]. The σ -algebra $\mathcal{A}$ is sufficient for the family of probability measures $\{v_t\}$ if the conditional expectation of any dynamical variable, say Hamiltonian $X(\omega)$ given the σ -algebra $\mathcal{A}$, that is, if $E\{X(\omega) | \mathcal{A}\}$ is the same for all $v_t \in \{v_t\}$ [3]. The sufficiency of the σ -algebra $\mathcal{A}$ implies the time-invariance of the conditional probability density $E\{\rho(\omega) | \mathcal{A}\}$ which by definition is our coarse-grained density under

consideration. The different non-null atoms of the sufficient σ -algebra a represent the different macrostates of statistical equilibria of the system at the initial time $t = 0$. This is a significant result. In an earlier paper [4], we have in fact shown that the sufficiency of the σ -algebra a for statistical equilibrium results from the ergodicity of the system.

The non-decreasing property of the entropy $\tilde{S}(v_t, a)$ is, however, not sufficient to ensure the relaxation to equilibrium over the phase-space (energy-shell) Ω . For this a more broad assumption, namely the assumption of mixing of phases is necessary. That the coarse-grained distribution generated by the σ -algebra a corresponds to the process of mixing results from the relation: $T_t a \supset a$. For measure-preserving automorphism T_t , the sequence $\{T_t a\}$ forms a monotonically increasing sequence of σ -algebra and let a_∞ where

$$a_\infty = \bigvee_{t=0}^{\infty} T_t a \quad (3.10)$$

be its limit in the sense that $T_t a \uparrow a_\infty$. Note the a_∞ being the smallest σ -algebra which includes all sets belonging to $T_t a$ ($t = 0, 1, 2, \dots$) is, therefore, equal to the σ -algebra $\{\phi, \Omega\}$, consisting of the null-set ϕ and the phase-space (ergodic set) Ω . Then by Doob's convergence theorem [5]

$$\lim_{t \rightarrow \infty} v\{A | T_t a\} = v\{A | a_\infty\} \quad (3.11)$$

which is the condition of weak-mixing or relaxation to statistical equilibrium [6]. To express it in a more familiar form we note that the σ -algebra $a_\infty = \{\phi, \Omega\}$ comprises of all sets of measure 0 and $m(\Omega)$. The mixing condition (3.11), then implies the convergence of the coarse-grained density $\bar{\rho}_t$ to the statistical equilibrium (microcanonical) density $1/m(\Omega)$:

$$\lim_{t \rightarrow \infty} \bar{\rho}_t = 1/m(\Omega) \quad (3.12)$$

or

$$\lim_{t \rightarrow \infty} \tilde{S}(v_t, a) = K \log m(\Omega) \quad (3.13)$$

where the r.h.s is the thermodynamic equilibrium entropy. Thus, while the ergodicity corresponds to the states of statistical equilibria over the various phase-cells (non-nullatoms of a) at the initial time $t = 0$, the mixing of phases ensures the limiting case of relaxation of the system to statistical equilibrium over the whole of phase-space Ω of the system.

4. CONCLUSIONS.

The paper aims to stress the importance of the properties of ergodicity and mixing in the coarse-grained interpretation of the irreversible approach to statistical equilibrium. The analysis is based on a measure of entropy defined for the non-equilibrium states of an isolated system. The invariance of the σ -algebra a under measure-preserving automorphism T_t corresponds to the statistical equilibria over the various phase-cells (including the whole phase-space Ω also) at the initial time $t = 0$. The sufficiency—a reduction principle of statistics, plays a significant role in the statistical characterization of statistical equilibria at the initial time. In the case of initial non-equilibrium distribution, it is, however, the assumption of phase-mixing which ensures the relaxation to statistical equilibrium over the whole of phase-space [4].

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