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Annals of Physics 320 (2005) 135–163

ANNALS of PHYSICS

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Generalized Gibbs ensembles for time-dependent processes

Ph. Chomaz [a,*], F. Gulminelli [b,1], O. Juillet [b]

[a] GANIL, DSM-CEA/IN2P3-CNRS, BP 5027, F-14076 CAEN cedex 5, France
[b] LPC Caen, IN2P3-CNRS et Université, F-14050 CAEN cedex, France

Received 17 December 2004; accepted 19 May 2005
Available online 14 July 2005

Abstract

An information theory description of finite systems explicitly evolving in time is presented for classical as well as quantum mechanics. We impose a variational principle on the Shannon entropy at a given time while the constraints are set at a former time. The resulting density matrix deviates from the Boltzmann kernel and contains explicit time odd components which can be interpreted as collective flows. Applications include quantum Brownian motion, linear response theory, out of equilibrium situations for which the relevant information is collected within different time scales before entropy saturation, and the dynamics of the expansion.

PACS: 05.70.Ln; 02.50.K; 89.70; 24.10.Pa

Keywords: Information theory; Non-equilibrium; Flows

1. Introduction

The microscopic foundations of thermodynamics are well established using the Gibbs hypothesis of statistical ensembles maximizing the Shannon entropy [1].When

* Corresponding author. Fax: +33 231454421.
[1] Member of the Institut Universitaire de France.

0003-4916/$ - see front matter
doi:10.1016/j.aop.2005.05.005

the thermodynamic limit can be taken, the various Gibbs ensembles for infinite systems converge to a unique thermodynamic equilibrium [28]. However, many systems studied in physics do not correspond to this mathematical limit of infinite systems [13] and, in fact, finite systems are now, per se, a subject of a very intense research activity, from metallic clusters [3,4] to Bose condensates [5,6], from nanoscopic systems [7] to atomic nuclei [8,9] and elementary particles [10]. The question thus arises: can the equilibrium of a finite systems be defined.

A priori, the Gibbs concept of statistical ensembles of replicas which is applicable for an arbitrary number of particles, seems an ideal tool to define the thermodynamics of finite systems. However, in a finite system the various Gibbs ensembles are not equivalent [11] and lead to different equilibria which physical meaning and relevance has to be investigated. In the different physical cases, which in the following encompass both the case of isolated systems and of systems in contact with a finite or infinite reservoir [29], the identification of the relevant statistical ensemble is a key issue.

From a macroscopic point of view, a common interpretation of a statistical ensemble is an infinite collection of infinite subsystems of the studied infinite system in a specific thermodynamic situation. The required independence of the different subsystems is insured by the thermodynamic limit. Within this interpretation, a single system can be considered as a statistical ensemble and thus can be discussed in terms of equilibrium. This kind of equilibrium is not relevant for a finite system since (i) the interface interactions between subsystem cannot be neglected, (ii) the procedure of coarse-graining modifies the entropic properties of the system, and (iii) a finite system does not lead to an infinite ensemble of subsystems. In fact a single realization of a finite system cannot be discussed in statistical physics terms.

An alternative viewpoint is given by the Boltzmann ergodic assumption. In this interpretation the statistical ensemble represents the collection of successive snapshots of a physical system evolving in time. The equivalence between this time average and the Gibbs ensemble is then insured by the ergodic theorem [30]. This interpretation however suffers from important drawbacks. First, not only a proof of the ergodic hypothesis under fairly general conditions is lacking, but even for a truly ergodic Hamiltonian, a finite time experiment may very well achieve ergodicity only on a subspace of the total accessible phase space [14]. Moreover, ergodicity applies to confined systems and thus it requires the definition of boundary conditions when the thermodynamic limit does not apply. Then the statistical ensemble in general explicitly depends on the boundary conditions and we will discuss in this article that an exact knowledge of the boundary corresponds to an infinite information and is therefore hardly compatible with the very principles of statistical mechanics, as a reduction of the many-body information to a (small) number of state variables.

Finally, in many physical situation the ergodicity ideas do not apply. Indeed, many physics experiments do not follow the time evolution of a single system, but rather concern averages over a great number of events, i.e., of physical replicas of systems experimentally prepared or sorted in similar way which are then observed at a given time. In such a context there is a priori no connection between the measuring time and the time it takes for an ergodic system to visit evenly the energy shell.