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Research paper

Ensemble inequivalence and Maxwell construction in the self-gravitating ring model

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ABSTRACT

The statement that Gibbs equilibrium ensembles are equivalent is a base line in many approaches in the context of equilibrium statistical mechanics. However, as a known fact, for some physical systems this equivalence may not be true. In this paper we illustrate from first principles the inequivalence between the canonical and microcanonical ensembles for a system with long range interactions. We make use of molecular dynamics simulations and Monte Carlo simulations to explore the thermodynamics properties of the self-gravitating ring model and discuss on what conditions the Maxwell construction is applicable.

1. Introduction

Equilibrium Statistical Mechanics is a hallmark of theoretical physics and an invaluable tool to study the properties of matter for more than a century. At its foundations lies Gibbs' ensembles theory [1], which is an elegant formulation applicable to a very broad class of phenomena (for a brief history of ensemble theory see [2]). As it is well known for any rounded practitioner, the microcanonical ensemble is harder to use than the canonical ensemble, and the grand-canonical ensemble is in a sense the more simple among them. Provided that the predictions of different ensembles coincide, one can then choose which one to use according to the needs in consideration. As a consequence, many authors devoted a considerable effort to the task of proving and establishing the limits of validity of the equivalence of the different ensembles (see [3] and references therein). From the thermodynamic viewpoint ensemble equivalence is based on the fact that the Legendre transformation connecting different ensembles is invertible. This implies particularly that the entropy is a concave function of the energy in the whole physically accessible energy range. In statistical terms it means that all properties of the system are well described either in terms of energy or temperature, that is essentially Gibbs' argument.

These respective ensembles are equivalent in the thermodynamic limit $N\rightarrow\infty$ if the interaction potential is tempered and stable, i. e. if the energy is additive and a stable equilibrium state exists [5]. The Helmholtz free energy and the grand-potential are then obtained from the microcanonical entropy by the usual Legendre transforms. Examples of physically relevant and non-stable potentials are the gravitational interaction, where for some specific cases the non-stability leads to the so-called gravothermal catastrophe [6], and multi-species plasmas [5]. As well known, equilibrium ensembles for self-gravitating systems are inequivalent, and an energy interval with negative heat capacity exists in the microcanonical ensemble [7]. The appearance of a convexity region in the entropy-energy curve breaks down the equivalence and any state

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of the system in the convex region cannot be realized in the canonical ensemble. The simplicity of Gibbs argument fails in this case [4].

According to van Hove's theorem [8], and under certain assumptions, the pressure P in the canonical ensemble must be a decreasing function of the volume V and becomes constant for the values of V in the interval of phase coexistence. In the microcanonical ensemble this corresponds to the Maxwell construction prescription to replace the entropy by its concave envelope. One of the conditions required in van Hove's theorem is that, for a three-dimensional system, the interparticle potential $V(r)$ satisfies $V(r) \geq r^{-3-\alpha}$ for $\alpha > 0$ and large distances r, i. e. that the potential is short-ranged and the total energy is additive. Therefore, in equilibrium statistical mechanics calculations, a convex intruder in the entropy function can only exist as a result of approximations, e. g. using a mean-field approach for a system with short-range interactions, or as a consequence of finite size effects [9–11]. This point is very well illustrated for the two-dimensional Potts model with nearest neighbors interaction, where a convex dip is present for small lattice size, disappearing for increasing N with the negative specific heat region being replaced by a flat curve, while for globally coupled spins, the convex dip remains even in the thermodynamic limit [12].

Thus the additivity of energy and entropy, which follows from the temperedness of the potential, and its stability, ensure that equilibrium ensembles are equivalent. The important point is that there exist real systems for which these conditions are not met. However, this does not imply that ensembles are not equivalent as the conditions are sufficient but not necessary.

Besides self-gravitating systems, examples of real physical situations with the occurrence of a convex intruder in the entropy are two-dimensional quasi-geostrophic flows [14], wave-particle interaction in a plasma in the presence of two harmonics [15,16] and magnetically self-confined plasma torus [17]. They also are examples of long-range interacting systems, with interacting potentials decaying at long-distances as $1/r^\alpha$ with $\alpha < D$, D being the spatial dimension [18–23]. This definition implies a non-additive energy as the interaction energy between two subsystems is no longer negligible when compared to the bulk energy. It is worth noticing that this definition may be at variance with some works in the literature, as for instance in Ref. [24] where an interaction with an exponential dependence on distance, and therefore not long-ranged in the sense adopted here, is referred as long-ranged.

The main goal of the present paper is to illustrate with a specific model of a many particle system with dynamics, for the first time up to the author's knowledge, the inequivalence of the microcanonical and canonical ensembles from first principles, i. e. by only solving the Hamilton equations of motion, and to show that the results so obtained are in agreement with previous theoretical studies and Monte-Carlos simulations. This allows us to discuss the physical origin of ensembles inequivalence as well as the meaning of the Maxwell construction if the interactions are long-ranged. The model system chosen is the one-dimensional self-gravitating ring model with Hamiltonian in Eq. (1), as its thermodynamic properties are well known, with a first order phase transition from a homogeneous to a non-homogeneous phase [25].

The structure of the paper is the following: the ring model is presented in Section 2 and in Section 3 we present our molecular dynamics results and compare them to Monte Carlo simulations and results from previous works. In Section 4 we discuss our results and present some concluding remarks.

2. The self-gravitating ring model

The self-gravitating ring (SGR) model was introduced by Sota and collaborators [25] and describes a system of N particles constrained to move on a circle and interacting by a gravitational potential regularized by a (usually small) softening parameter ϵ introduced in order to avoid the divergence of the potential at short distances. With a proper choice of units its Hamiltonian can be written as:

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} - \frac{1}{2N} \sum_{i,j=1}^{N} \frac{2\sqrt{\epsilon}}{\sqrt{1-\cos(\theta_i-\theta_j)+\epsilon}}, \qquad (1)$$

with θ_i being the position angle on the circle of particle i and p_i its conjugate (angular) momentum. Here units have been chosen such that the minimum value of the energy per particle is -1 irrespective of the value of ϵ. The factor $1/N$ in the potential energy term is known as the Kac factor, and can be introduced by a change of time units (as long as N remains finite), in order for the total energy to be extensive, although remaining non-additive. It also facilitates the comparison of results with different numbers of particles. The analogous of a magnetization can be introduced here by its components:

$$M_x = \frac{1}{N}\sum_{i=1}^{N}\cos\theta_i, \qquad M_y = \frac{1}{N}\sum_{i=1}^{N}\sin\theta_i. \qquad (2)$$

Many properties of the model were studied in previous works [26–31]. It has a phase-transition from a low energy ferromagnetic phase to a high energy homogeneous (non-magnetic) phase. The order of the transition depends on the value of the softening parameter. For smaller values of ϵ the transition is first order and becomes continuous for higher values of the parameter. It is worth noticing that for systems with long-range interaction in the $N \to \infty$ limit particles are exactly uncorrelated [32].