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Physica A 359 (2006) 447–454
PHYSICA A
www.elsevier.com/locate/physa

Topological approach to phase transitions and inequivalence of statistical ensembles

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Received 3 June 2005
Available online 20 July 2005

Abstract

The relation between thermodynamic phase transitions in classical systems and topology changes in their state space is discussed for systems in which equivalence of statistical ensembles does not hold. As an example, the spherical model with mean field-type interactions is considered. Exact results for microcanonical and canonical quantities are compared with topological properties of a certain family of submanifolds of the state space. Due to the observed ensemble inequivalence, a close relation is expected to exist only between the topological approach and *one* of the statistical ensembles. It is found that the observed topology changes can be interpreted meaningfully when compared to microcanonical quantities.

Keywords: Phase transitions; Topology; Ensemble inequivalence; Spherical model

Phase transitions, like the boiling and evaporating of water at a certain temperature and pressure, are common phenomena both in everyday life and in almost any branch of physics. Loosely speaking, a phase transition brings about a sudden change of the macroscopic properties of a system while smoothly varying a parameter (the temperature or the pressure in the above example). For the description of equilibrium phase transitions within the framework of statistical mechanics, several so-called statistical ensembles or Gibbs ensembles, like the

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doi:10.1016/j.physa.2005.06.063

microcanonical or the canonical one, are at disposal, each corresponding to a different physical situation. For a large class of systems with sufficiently short ranged interactions, these different approaches lead to identical numerical values for the typical system observables of interest, after taking the thermodynamic limit of the number of particles in the system going to infinity [1]. In this situation one speaks of equivalence of ensembles. Then, instead of selecting the statistical ensemble according to the physical situation of interest, one can revert to the ensemble most convenient for the computation intended. For systems with long range interactions, however, equivalence of ensembles does not hold in general. Systems showing such an inequivalence of ensembles in the thermodynamic limit (among those gravitational systems and Bose–Einstein condensates) have attracted much research interest in the last years (see Ref. [2] for a review). Dramatic differences between the ensembles can be observed for example in the specific heat, which is a strictly positive quantity in the canonical ensemble, whereas, negative values, and even negative divergences, can occur in the microcanonical ensemble [3,4].

An entirely different approach to phase transitions, not making use of any of the Gibbs ensembles, has been proposed recently. This *topological approach* connects the occurrence of a phase transition to certain properties of the potential energy V, resorting to *topological* concepts. From a conceptual point of view, this approach has a remarkable property: the microscopic Hamiltonian dynamics can be linked via the Lyapunov exponents to the topological quantities considered [5]. With the topological approach, in turn, linking a change of the topology to the occurrence of a phase transition, a concept is established which provides a connection between a phase transition in a system and its underlying microscopic dynamics.

The topological approach is based on the hypothesis [6] that phase transitions are related to topology changes of submanifolds Σ_v of the state space of the system, where the Σ_v consist of all points q of the state space for which $V(q)/N = v$, i.e., their potential energy per degree of freedom equals a certain level v. (Or, in a related version, the topology of submanifolds M_v consisting of all points q with $V(q)/N \leqslant v$ is considered.) This hypothesis has been corroborated by numerical and by exact analytical results for a model showing a first-order phase transition [7,8] as well as for systems with second-order phase transitions [5,9–13]. A major achievement in the field is the recent proof of a theorem, stating, loosely speaking, that, for systems described by smooth, finite-range, and confining potentials, a topology change of the submanifolds Σ_v is a *necessary* criterion for a phase transition to take place [14].

Albeit necessary, such a topology change is clearly not *sufficient* to entail a phase transition. This follows for example from the analytical computation of topological invariants in the XY model [9,10], where the number of topology changes occurring is shown to be of order N, but only a single phase transition takes place. So topology changes appear to be rather common, and only particular ones are related to phase transitions. There are strong indications that a criterion based exclusively on topological quantities cannot exist in general [13].

Having mentioned the recent efforts to more firmly establish sufficient and necessary relations between topology changes and phase transitions, and bearing in mind the phenomenon of ensemble inequivalence, we notice an additional