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Singular behavior of fluctuations in a relaxation process

Federico Corberi [a,*], Giuseppe Gonnella [b], Antonio Piscitelli [c]

[a] Dipartimento di Fisica "E.R. Caianiello", and CNISM, Unità di Salerno, Università di Salerno, via Ponte don Melillo, 84084 Fisciano (SA), Italy
[b] Dipartimento di Fisica, Università di Bari and INFN, Sezione di Bari, via Amendola 173, 70126 Bari, Italy
[c] Division of Physical Sciences, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link, 637371 Singapore, Singapore

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ABSTRACT

Carrying out explicitly the computation in a paradigmatic model of non-interacting systems, the Gaussian model, we show the existence of a singular point in the probability distribution $P(M)$ of an extensive variable M. Interpreting $P(M)$ as a thermodynamic potential of a dual system obtained from the original one by applying a constraint, we discuss how the non-analytical point of $P(M)$ is the counterpart of a phase-transition in the companion system. We show the generality of such mechanism by considering both the system in equilibrium or in non-equilibrium state following a temperature quench.

1. Introduction

Phase transitions are described by thermodynamic functions displaying singular behavior. For many complex systems, like inhomogeneous or disordered systems, the basic mechanisms of phase transitions are still under debate. On the other hand, there is a large class of systems where the occurrence of a phase-transition can be ascribed to the existence of a constraint, acting as an effective interaction for otherwise independent variables. For instance, it is well known that in bosons with an unrestricted number, as photons or phonons, phase transitions do not show up. But the situation changes radically when particles with a conserved number are considered, leading to the remarkable phenomenon of the Bose–Einstein condensation (BEC) [1]. The condensation mechanism, with a certain sector of the phase space (the zero wavevector model in BEC) becoming macroscopically populated, is typical of phase transition in constrained systems. Another worth example is provided by the Spherical model of Berlin and Kac [2], obtained by constraining the order parameter field of the Gaussian model on a hypersphere of radius S[2,3]. While the Gaussian model is paradigmatic of a non-interacting system [4] with well-known trivial equilibrium properties, the Spherical model shows a highly non-trivial behavior, characterized by a second-order phase transition in $d = 3$.

Constraints also appear in a conceptually different context, when one wants to evaluate the probability of observing an extremely unlikely value M of a macrovariable $\mathcal{M}$, as for instance the energy in a canonical setting, due to a rare fluctuation of a thermodynamic system. Loosely speaking, in a sense that finds a clear explanation in the context of the *large deviation theory*[5] and that will better qualified in Section 2, the measurement of such probability can be regarded as a constraint applied on the system, since this basically amounts to keep the configurations where the constraint $\mathcal{M} = M$ is fulfilled, discarding the others. Then, recalling the previous discussion, even if the average properties of the system under study are trivial, it can appear not surprising that the measurement of the probability distribution of some of its macrovariables may show singular points. However, only very recently, the occurrence of singularities in the large deviation functions of a number of different models has been recognized [6–11] and interpreted in terms of a condensation mechanism.

Recently [12], we have studied the occurrence of a non-analytical behavior in the probability distribution of macrovariables in the context of the Gaussian model. Choosing $\mathcal{M} = \mathcal{S}$, the order parameter variance, this amounts to impose the Berlin–Kac constraint, as said above. The purpose of this paper is, after reviewing some of the results of [12], to discuss the singular behavior of the probability distribution of $\mathcal{S}$ not only in equilibrium but also, by considering the relaxation following a temperature quench, in the largely unknown area of the non-equilibrium processes without time translation invariance [13,14].

The paper is organized as follows: In Section 2 we describe on general grounds the relation between the probability of fluctuations of macrovariables and the application of a constraint and, in Section 2.1, how such probabilities can be computed by saddle point techniques in the large-volume limit. The Gaussian model is introduced in Section 3. This is the central section of the paper, where the probability distribution of a particular macrovariable is explicitly determined (Sections 3.1, 3.2) and its non-analytical behavior is discussed (Section 3.3). This leads to

* Corresponding author.
E-mail addresses: corberi@sa.infn.it (F. Corberi), gonnella@ba.infn.it (G. Gonnella), AntPs@ntu.edu.sg (A. Piscitelli).

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the determination of a phase-diagram, namely the parameter region where condensation of fluctuations occurs, in Section 3.4. Finally, in Section 4 we conclude by a discussion of some open points and the perspectives of future research on the subject.

2. Probability distributions of macrovariables and constraints

Let us consider a thermodynamic system whose microscopic degrees of freedom we denote by $\varphi = \{\varphi_i\}$, where i labels each of such variables. For instance, $\varphi_i \equiv \vec{s}_i$ could be the spin on the sites i of a lattice in the case of a magnetic system.

Let $P(\varphi, J)$ be the probability distribution of the microstates in the presence of certain control parameters J, such as volume and temperature and, if the system is not in equilibrium, time. A generic random variable, like the energy of the system in contact with a bath, is a function $\mathcal{M}(\varphi)$ of the representative point in the phase-space Ω. The probability to observe a certain value M of such fluctuating quantity can be formally written as

$$P(M, J) = \int_\Omega d\varphi P(\varphi, J)\delta(M - \mathcal{M}(\varphi)). \tag{1}$$

In the case of equilibrium states, the expression on the r.h.s. of this equation can be readily interpreted as the partition function of a new system, whose microstates φ occur with probability

$$P(\varphi, M, J) = \frac{1}{P(M, J)} P(\varphi, J)\delta(M - \mathcal{M}(\varphi)). \tag{2}$$

This system is obtained from the original one by fixing

$$\mathcal{M}(\varphi) = M. \tag{3}$$

This constraint could be, in specific examples, the conservation of the number of particles in a bosonic gas or the restriction on the hypersphere of the order-parameter field in the Spherical model.

Moving the value of M it may happen that a critical point M_c is crossed in the constrained model. Resorting again to the previous examples, by fixing all the other control parameters (among which temperature), BEC is observed upon raising the free boson number above a certain value, or the ferromagnetic phase is entered in the Spherical model when the hypersphere radius exceeds S_c.

If this happens, the partition function of the constrained model will be singular at criticality and, because of Eq. (1), a point of non-analyticity will be found in the probability distribution $P(M, J)$ of the fluctuating variable $\mathcal{M}$.

So far we have discussed the case of equilibrium states, where the r.h.s. of Eq. (1) can be interpreted as the partition function of a restricted model. If the system is not in equilibrium, this expression is not amenable of the same interpretation. Nevertheless a singularity can still be produced by a mechanism which resembles a dynamical phase-transition, as it will be shown in Section 3.4.

2.1. Large volume limit

Introducing the integral representation of the δ function $\delta(x) = \int_{\alpha-i\infty}^{\alpha+i\infty} \frac{dz}{2\pi i} e^{-zx}$, Eq. (1) becomes

$$P(M, J) = \int_{\alpha-i\infty}^{\alpha+i\infty} \frac{dz}{2\pi i} e^{-zM} K_\mathcal{M}(z, J) \tag{4}$$

where

$$K_\mathcal{M}(z, J) = \int_\Omega d\varphi P(\varphi, J) e^{z\mathcal{M}(\varphi)} \tag{5}$$

is the moment generating function of $\mathcal{M}$. If the system is extended and $\mathcal{M}(\varphi)$ is an extensive macrovariable, for large volume Eq. (4) can be rewritten as

$$P(M, J, V) = \int_{\alpha-i\infty}^{\alpha+i\infty} \frac{dz}{2\pi i} e^{-V[zm + \lambda_\mathcal{M}(z,J)]} \tag{6}$$

where we have explicitly separated the volume V from the bunch of control parameters J, m is the density M/V and

$$-\lambda_\mathcal{M}(z, J) = \frac{1}{V} ln K_\mathcal{M}(z, J, V) \tag{7}$$

is volume independent in the large-volume limit. Carrying out the integration by the saddle point method one arrives at

$$P(M, J, V) \sim e^{-V I_\mathcal{M}(m,J)} \tag{8}$$

with the rate function

$$I_\mathcal{M}(m, J) = z^* m + \lambda_\mathcal{M}(z^*, J) \tag{9}$$

and where $z^*(m, J)$ is the solution, supposedly unique, of the saddle point equation

$$\frac{\partial}{\partial z} \lambda_\mathcal{M}(z, J) = -m. \tag{10}$$

Eq. (8) amounts to the large deviation principle, according to which the probability of a fluctuation of a macrovariable is exponentially damped by the system volume with rate function $I_\mathcal{M}(m, J)$.

3. A specific example: the Gaussian model

As a simple, fully analytical model to test the above ideas the Gaussian model was considered in [12]. The set of microvariables are represented by a scalar order parameter field $\varphi(\vec{x})$, governed by the bilinear energy functional

$$H[\varphi] = \frac{1}{2} \int_V d\vec{x} \left[(\nabla\varphi)^2 + r\varphi^2(\vec{x}) \right] \tag{11}$$

where r is a non-negative parameter. In order to study both the equilibrium behavior and the non-equilibrium process where time translational invariance is spoiled we consider a protocol where the system is kept in equilibrium at the temperature T_I at times $t < 0$. Then, at the time $t = 0$ it is instantaneously quenched to the lower temperature T_F. The dynamics, without conservation of the order parameter, is governed by the overdamped Langevin equation (Ref. [4])

$$\dot{\varphi}(\vec{x}, t) = \left[\nabla^2 - r \right] \varphi(\vec{x}, t) + \eta(\vec{x}, t) \tag{12}$$

where $\eta(\vec{x}, t)$ is the white Gaussian noise generated by the cold reservoir, with zero average and correlator

$$\left\langle \eta(\vec{x}, t)\eta(\vec{x}', t') \right\rangle = 2T_F \delta(\vec{x} - \vec{x}')\delta(t - t'), \tag{13}$$

where we have set to unity the Boltzmann constant. Due to linearity, the problem can be diagonalized by Fourier transformation. For the Fourier components $\varphi_{\vec{k}} = \int_V d\vec{x} \varphi(\vec{x}) e^{i\vec{k}\cdot\vec{x}}$, by imposing periodic boundary conditions, one gets the equations of motion

$$\dot{\varphi}_{\vec{k}}(t) = -\left(k^2 + r\right)\varphi_{\vec{k}}(t) + \eta_{\vec{k}}(t) \tag{14}$$