ISING MODEL WITH TWO TEMPERATURES:
SIMULATION AND THEORY

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ABSTRACT

We present here both a Monte Carlo (MC) simulation and a Fokker-Planck equation (FPE) approach to the kinetic Ising model with two competing temperatures[1]. The MC simulation of this non-equilibrium model shows that its macroscopic stationary properties are very sensitive to the analytical form of the microscopic dynamical mechanism. Taking into account the MC results we derive different FPE by using standard techniques. The deficiences of each of these FPE are discussed and one of them is found to be the most suitable in order to treat the model in a field theoretical context.

1. Introduction

Field theoretical methods have proved very useful in the study of equilibrium phase transitions; in particular, they have allowed to clarify the concepts of scaling and universality, and to obtain the values of critical exponents both in static and dynamical problems. An extension of these ideas to deal with nonequilibrium problems is presently of great interest. The model that we study here is the kinetic Ising model with two temperatures [1]. It simulates the presence of two thermal baths acting on a magnetic system. This model is a non-equilibrium one because of the presence of *dynamical frustration*, i. e., due to the competition between different dynamical mechanisms (each one characterized by a different temperature) the detailed balance condition does not hold and it does not seem possible to express the stationary solution as a Gibbs distribution. Since no exact method is available to solve this model a computer simulation has been carried out.

The simulation shows that contrarily to what happens in equilibrium problems, in this model there is a dependence of the macroscopic stationary properties on the analytical form of the microscopic dynamical mechanism (i.e. on the concrete realization of the master equation that defines the model)[2]. Therefore, any description of this model should take into account this dependence. In particular, the starting point for a field theoretical approach to a kinetic model is the so-called

Fokker-Planck Equation (FPE). Then, the latter equation has to contain sufficient microscopic kinetic information to properly describe the macroscopic behavior of the system.

The paper is divided in two parts. In the first one the model is defined and the MC simulation is described. In the second one we introduce different FPE which have been derived by using standard techniques. We discuss their shortcomings and select the most suitable to achieve our goals.

2. The Model and the MC simulation

Let us consider a dynamical Ising model in two dimensions with a total of ν spin variables $s_x = \pm 1, x \in \Lambda$ and Λ being a square lattice. The evolution of the system is governed by a markovian master equation in which only spin flip processes are considered:

$$\partial_t P(s,t) = \sum_x (w(s^x,x)P(s^x,t) - w(s,x)P(s,t)) \tag{1}$$

where s is a spin configuration, $P(s,t)$ is the probability of finding the system in s at a given time t, s^x is the configuration obtained by flipping the spin at x in s, and $w(s,x)$ is the probability per unit time for the transition from the configuration s to s^x.

For systems whose stationary state is an equilibrium one defined by a Hamiltonian $H(s)$, the rates, $w(s,x)$, that fulfil the detailed balance condition:

$$w(s,x)\exp(-\beta H(s)) = w(s^x,x)\exp(-\beta H(s^x)) , \tag{2}$$

guarantee that the system will evolve from almost all initial conditions to its final equilibrium state. Besides, it is usual to consider $w(s,x)$ depending only upon the variation of $H(s)$ in the transition. The rates verifying the latter two conditions can be written as: $w(s,x) = \varphi(\beta \delta H(s))$, where $\delta H = H(s^x) - H(s)$ and $\varphi(z) = e^{-z}\varphi(-z)$. For example, two usual choices are: (i) $\varphi(z) = exp(-z/2)$ and (ii) $\varphi(z) = 1 - tanh(z/2)$. For a fixed Hamiltonian, the stationary properties of these models does not depend on the concrete form of $\varphi(z)$.

The kinetic Ising model with two competing temperatures consists on having a rate which is the superposition of two different mechanisms: $w(s,x) = pw_1(s,x) + (1-p)w_2(s,x)$. Each $w_j, j = 1,2$, when acting apart, drives the system to a different equilibrium distribution, $P_{st,j}(s) = exp(-\beta_j H_{Ising}(s))/Z$ where β_j is the inverse of the jth temperature, $H_{Ising} = -J\sum_{|x-y|=1} s_x s_y$ and $0 \leq p \leq 1$. In dimension greater than one, the competition between both mechanisms prevents the system to fulfil a detailed balance condition with respect to any hamiltonian. As a consecuence, the stationary solution of the master equation will be a non equilibrium one.

In order to gain insight about the behavior of this system we have performed a MC simulation. We have taken a 96*96 lattice and considered two kinds of transition rates commonly used in the literature, namely, the ones given by (i) and (ii) above. The values of p and T_1 are maintained fixed in each simulation and T_2

is varied. We will not present here a detailed analysis of the simulations, but only expose the main qualitative results:

1- The curves of the net magnetization m versus T_2 have different shapes for different rates. In particular $m(T_2 = 0) = \pm 1$ and $|m(T_2 = 0)| < 1$ for the defined above rates (i) and (ii) respectively. Different behaviors are also found for the energies, specific heats, susceptibilities, and other magnitudes when the transition rates are modified. The differences are, as in the net magnetization case, both quantitative and qualitative.

2- When T_1 is close to the Onsager temperature, T_O, the system can be described quite well like an equilibrium one, with an effective temperature.

3- Although our results in this respect are not conclusive, it seems that the slopes of the magnetization curves at the critical point differ from the equilibrium one, and they also depend on the parameters as p or T_1. Thus, critical exponents may change. Futher simulations are required in order to better elucidate this point.

The main conclusion is that the analytical form of the transition rates influences dramatically the macroscopic behavior of the system.

3. Fokker Planck Equations (FPE)

As we have pointed out before, a field theoretical approach for this model, requires a FPE describing it as reliably as possible. There are different ways to approximate a given master equation by a FPE; none of them is rigorous, but it is possible to impose several conditions to the FPE that can make it much more reliable.

A usual way to get a FPE in equilibrium dynamical problems consists of replacing the original microcopic dynamical model by a continuous simpler one in such a way that the global properties of the stationary state, i.e. symmetries, phase transitions and criticallity.., are maintained. This is the case of the model A used to study dynamical properties of the non-conservative Ising model [3]. The success of this substitution in the study of equilibrium critical phenomena is guaranteed because of universality. In our nonequilibrium problem we can define a FPE in a similar way: the simplest one we can construct consists of the superposition of two models A, each of them with a different temperature. In this same level of aproximation we can also consider some approaches for driven diffusive systems[4], that are also non-equilibrium problems, but where the system is approximated by a modified model B[3]. This is in principle an oversimplification because the dependence on the microscopic dynamics is played down. Universality in nonequilibrium critical phenomena has not been proved in general. So, the construction of a FPE in the way described above is at least dangerous. We cannot guarantee that the critical behavior of our original model is the same that the one generated in this approximation. In fact, as it can be easily shown, this way to proceed reduces the problem to an effective equilibrium one, that is, the system behaves as if it were at equilibrium with an effective temperature defined by $T_{eff} = pT_1 + (1 - p)T_2$, and any other nonequilibrium effect, such as the dependence on the dynamics, is

eliminated. This is in disagreement with what we observe in the MC simulation. Therefore the conclusion is that, as this kind of simplifications is not safe enough, in order to represent the system we need a more elaborated FPE that should describe the original model as closely as possible.

A second way to derive a continuous FPE is provided by truncating a Kramers Moyal expansion of the original master equation [5]. This standard approach respects a dependence on the microscopic dynamics, but it presents important deficiences. In particular, a disadvantage of this approach is that the detailed balance condition does not hold even in the equilibrium case, and so this form to do the continuum limit does not maintain the property that the stationary solution is an equilibrium one. This is a very dissapointing fact because even in the simplest case of systems at equilibrium spurious phenomena may appear. So we consider that this approach is not good enough for our purposes.

In order to overcome these drawbacks, we have derived a new FPE following the scheme introduced by Hanggi et al [6] which guarantees that, in the continuum limit, the stationary solutions for systems with equilibrium states is preserved. The FPE derived is:

$$\frac{\partial P(\phi;t)}{\partial t} = -\int dx \left[\frac{\delta}{\delta\phi(x)} a[\phi(x)] + \frac{1}{\nu} \frac{\delta}{\delta\phi(x)} L[\phi(x)] \frac{\delta}{\delta\phi(x)} \right] P(\phi, t) \tag{5}$$

where $\phi(x)$ is the continuous magnetization at point x. The coefficients $a_1(\phi, x)$ and $L(\phi, x)$, whose definition will be given elsewhere [7], depend on the concrete form of the transition rates. This FPE reproduces in the equilibrium limit the exact stationary solution and depends on the microscopic dynamics in nonequilibrium cases. Therefore it constitutes a convenient starting point to apply field theoretical techniques [8] to our model. In particular, starting from this FPE it is possible to derive the solution in a path integral form with an asociated lagrangean density which depends on the dynamics. This is the basis to renormalize the theory, to consider renormalization group techniques and to study, for example, the critical exponents of the system.

In conclusion, we have pointed out that the role of microscopic dynamics is essential in a non-equilibrium system and we have derived a suitable FPE to include properly this fact in a field theoretical treatment.

References

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