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Phase behavior under the averaging over disorder realizations

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ABSTRACT

Effects of the averaging over disorder realizations (samples) on the phase behavior are analyzed in terms of the mean field approximation for the random field Ising model with infinite range interactions. It is found that the averaging is equivalent to a drastic modification in the statistics of the quenched variables. In its turn, this lowers the critical temperature of a second-order phase transition or, depending on the sampling, even suppresses the ordered phase. Possible first order transitions are shown to be softened by the sample averaging. Common issues and differences in the interpretation of these effects in the context of the simulation and experimental studies are discussed.

1. Introduction

An influence of a quenched disorder on the phase behavior is a long-standing problem that has received much interest [1,2]. Various theoretical aspects, such as disorder relevance, Griffiths phenomena, possible lack of self-averaging [3] or disorder-induced rounding are being discussed [4] (see Ref. [5] for a recent review). In the case of the so-called weak (or random T_c) disorder it is believed [5] that the details of the probability distribution should not be important because the physics is dominated by the long-range properties.

On the other hand, there are systems in which the shape of the probability distribution is important. For instance, the fluid adsorption [6] or the colloid-polymer mixtures separation in random porous media are found [7] to belong to the universality class of the random-field Ising model (RFIM) [1,8]. The latter is just a prototype of a system, where the randomness plays an essential role, the so-called strong disorder [9]. In contrast to the weak disorder case [4,5], a change in the distribution modifies the degree of frustration, inducing specific fluctuations [10], which are not present in the pure (bulk) case. The RFIM has been analyzed in the mean field approximation (MFA) [11–13] and more recently by computer simulations [10,14]. The distribution width [11], asymmetry [12] or bimodality [13,15,16] have been shown to induce crucial changes in the phase diagram. Nevertheless, in the context of adsorption studies it becomes questionable [6,17] that the true equilibrium picture is observed in experiments, revealing a hysteretic behavior instead of sharp steps typical for a two phase coexistence. Moreover, it has been demonstrated [6,18] that the hysteresis can exist even without an underlying phase transition. This, however, does not discard completely a possibility of the phase behavior in disordered systems, but rather makes one to search for the conditions at which it can be observed.

Another aspect of the randomness is that two quenched systems prepared in the same way are not microscopically identical because only few macroscopic disorder parameters are usually controlled. Therefore, one has to average over different realizations. In the present study we argue that in this class of systems the averaging over disorder realizations in the

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simulations or appearing in the context of self-averaging hypothesis [1,2] in the analysis of experiments, is equivalent to crucial changes in the distribution of quenched variables (random fields in the RFIM language). In this way a sample averaged distribution brings up new statistical features which are absent from the statistics of each sample. Consequently, the phase behavior seen on average can be remarkably different from that in a separate sample. In particular, we are going to analyze whether a small difference of realizations can lead to qualitative changes in the phase behavior.

2. Averaging in disordered systems

Let us consider a quenched-annealed system. The annealed subsystem consists of interacting species (e.g. particles or spins) characterized by a set of variables $\{s_i\}$. The latter are governed by some Hamiltonian $H[\{s_i\}|\{h_k\}]$ that contains a set of quenched variables (local porosities or magnetic fields) $\{h_k\}$, distributed according to some probability density $f(\{h_k\})$. For simplicity we assume the disorder to be non-correlated $f(\{h_k\}) = \prod_k f(h_k)$, such that the position label is dropped $f(h_k) = f(h)$. In contrast to coupled annealed systems (e.g. an adsorbate–substrate coupling [19]), in quenched-annealed systems the averaging should be taken in two steps. Tracing off the annealed variables one gets a quenched thermodynamic function $m(h)$ (an order parameter) that is conditional to the state, h, of the quenched counterpart. Then, as usually [1,2], one takes an average of $m(h)$ with the distribution $f(h)$.

However, in reality, the situation is not so straightforward. In experimental or simulation studies only few disorder parameters (e.g. mean porosity, average field or site activity) are usually controlled during the quenching. Therefore, one has to deal with sample-to-sample fluctuations in different realizations r. Thus, for a given sample the distribution implicitly depends on the realization $f(h) = f(h|r)$. Consequently, the disorder averages are also realization dependent:

$$m(r) = \overline{m(h)} = \int \mathrm{d}h f(h|r) m(h). \tag{1}$$

In order to find a "representative" result in the simulations one could generate an ensemble of samples corresponding to different realizations which appear with a probability density $\varphi(r)$. Such a procedure has recently been reported [20]. Then an average over realizations is taken:

$$m = \int \mathrm{d}r \varphi(r) m(r) = \int \mathrm{d}r \varphi(r) \int \mathrm{d}h f(h|r) m(h). \tag{2}$$

If the sampling $\varphi(r)$ does not depend on the h-disorder, we may change the order of integration, defining the realization-averaged (or sample-averaged) distribution

$$\Psi(h) = \int \mathrm{d}r \varphi(r) f(h|r). \tag{3}$$

Then the order parameter should be calculated from

$$m = \int \mathrm{d}h \Psi(h) m(h). \tag{4}$$

On the other hand, an experimentalist is usually working with a single system (or with few systems). This rises a question on a representability of a single experiment for a given class of materials. This leads to the concept of self-averaging [1–3,5]. Namely, it is assumed that an experimental system is large enough, such that it may be viewed as a composition of a large number of macroscopic subsystems (samples). Each of them corresponds to a different realization of the quenched disorder. In this way a measurement corresponds to an average over the subsystems, thus we arrive at the same representation (3), (4). This mathematical similarity enables one to compare the simulation and the experimental results. Note that the averaging over realizations (3) is formally equivalent to creating some "representative" or "typical" [1] sample with a distribution $\Psi(h)$ that is thought to incorporate the generic features, independent of the system preparation procedure. However, in the context of experimental studies, invoking the self-averaging concept, this system is (or is believed to be) a real object, while in the simulation, where each realization can be tested independently, it is artificial.

Therefore, despite its logical transparency, the averaging (3) is not a trivial procedure. It leaves some important questions, such as how the final result (4) depends on the sampling $\varphi(r)$ and on the quenching in each sample $f(h|r)$? Indeed, from Eq. (3) we may expect that, depending on these ingredients, the resulting distribution $\Psi(h)$ could be remarkably different from that in a separate sample. From a quite general point of view this issue has been analyzed within the superstatistical approach [21]. It has been demonstrated how an exponential distribution (e.g. of Boltzmann type) transforms into a power-law as a result of a fluctuating environment [21,22] or a constraint [23] restricting the phase space. In its turn, such a modification in the statistics of the quenched variables (namely, an enhancement of "rare" events [4,5,9]) might lead to non-trivial consequences for the thermodynamics, especially near a phase transition point. In what follows we analyze this issue in more detail.

3. Phase behavior

Realizations of the quenched subsystem are usually obtained by repeating some preparation procedure (e.g. sol–gel technique in experiments, or diffusion-limited aggregation in the simulation studies). Therefore, it is reasonable to accept