Available online at www.sciencedirect.com
ScienceDirect
ELSEVIER
Physica A 387 (2008) 2256–2266
PHYSICA A
www.elsevier.com/locate/physa

Monte Carlo analysis of critical properties of the two-dimensional randomly site-diluted Ising model via Wang–Landau algorithm

I.A. Hadjiagapiou*, A. Malakis, S.S. Martinos

Section of Solid State Physics, Department of Physics, University of Athens, Panepistimiopolis, GR 15784 Zografos, Athens, Greece

Received 5 December 2007
Available online 14 December 2007

Abstract

The influence of random site dilution on the critical properties of the two-dimensional Ising model on a square lattice was explored by Monte Carlo simulations with the Wang–Landau sampling. The lattice linear size was $L = 20$–120 and the concentration of diluted sites $q = 0.1, 0.2, 0.3$. Its pure version displays a second-order phase transition with a vanishing specific heat critical exponent α, thus, the Harris criterion is inconclusive, in that disorder is a relevant or irrelevant perturbation for the critical behaviour of the pure system. The main effort was focused on the specific heat and magnetic susceptibility. We have also looked at the probability distribution of susceptibility, pseudocritical temperatures and specific heat for assessing self-averaging. The study was carried out in appropriate restricted but dominant energy subspaces. By applying the finite-size scaling analysis, the correlation length exponent ν was found to be greater than one, whereas the ratio of the critical exponents (α/ν) is negative and (γ/ν) retains its pure Ising model value supporting weak universality.

PACS: 05.50.+q; 75.10.Hk; 05.10.Ln; 64.60.Fr

Keywords: Lattice theory; Two-dimensional Ising model; Randomness; Site dilution; Monte Carlo; Wang–Landau; Finite-size scaling

1. Introduction

In the last few years, many theoretical, numerical and experimental investigations have appeared for the study of the influence of disorder (usually quenched site or bond dilution) on statistical systems in the presence or absence of an external magnetic field, since an experimental sample is not free of disorder, in general. Such systems are randomly dilute uniaxial antiferromagnets, e.g. $Fe_qZn_{1-q}F_2$, $Mn_qZn_{1-q}F_2$, $Fe_{1-q}Al_q$, obtained by mixing uniaxial antiferromagnets with nonmagnetic materials. These systems are modelled by using pure systems models modified accordingly. The most popular models for pure systems are those of Ising and Potts; in the current case, the former one shall be used.

The Ising model, a favourite for physicists, is used as the prototype for phase transitions, critical phenomena, biological and econophysics, owing to the fact that its two-dimensional version on a square lattice was solved

* Corresponding author. Tel.: +30 2107276771; fax: +30 2107276711.
E-mail address: ihatziag@phys.uoa.gr (I.A. Hadjiagapiou).

0378-4371/$ - see front matter
doi:10.1016/j.physa.2007.12.007

analytically by Onsager, [1]; it has also become a standard model for testing scaling and universality hypotheses. The Ising model as well as that of Potts, Heisenberg, Baxter-Wu, etc. represent collective phenomena which are difficult to be solved exactly, except in some cases, consequently approximate methods have been developed to cope with, such as mean field theory, numerical methods, perturbation theory, scaling, renormalization group, Monte Carlo, etc. The effect of randomness on the critical behaviour and magnetic phase diagrams of classical random spin systems has attracted much interest in recent years. Randomness is encountered in the form of vacancies, variable bonds, impurities, random fields, etc. Its influence on the critical behavior and magnetic properties is a long-standing and still unsettled problem in statistical physics. Similar methods, as in the pure systems, have been utilized for the study of these systems. In these studies, an important question which had arisen was the extent to which randomness influences the critical behaviour and magnetic properties. The first remarkable criterion for the influence of randomness on a critical system was proposed by Harris, [2], according to which randomness changes the critical behaviour if the specific heat critical exponent α of the pure system is positive, $\alpha > 0$. In this case a new critical point with conventional power law scaling and new exponents emerges. However, the pure two-dimensional Ising model (2D IM) constitutes a marginal situation since $\alpha = 0$. This exception makes 2D IM of particular interest attracting much attention. However, this effort led to contradicting results, increasing confusion and revealing the inhibit hidden complexity, implying the need for more subtle approaches to tackle it.

The 2D IM consists of an array of N fixed points lying on the sites of a two-dimensional lattice of linear size L such that $N = L^2$. Each lattice site is occupied by a magnetic atom characterized by the spin variable S_i, $i = 1, 2, \ldots, N$, with S_i taking on the values ± 1. One can also consider a modified version of this model wherein some of the lattice sites, chosen randomly, are either vacant or occupied by nonmagnetic atoms, (e.g. Al atoms [3]); both cases of randomness are treated equivalently. This version of Ising model is called two-dimensional randomly site-diluted Ising model (2D RSDIM). For this system, the critical exponents associated with the random fixed point have been estimated for the dilution-type disorder by theoretical and numerical approaches, leading to questionable conclusions, [4]. However, these approaches have shed light on estimates of the critical temperature and nature of the phase transition. In addition, the phase diagram is strongly influenced, among other factors, by dilution, [5]. The concentration of vacancies (or nonmagnetic particles) is denoted by q (dilution), while that of occupied sites (magnetic particles) by p (purity), $q + p = 1$. The vacancies are considered to be quenched and uncorrelated, since one can also encounter systems where the vacancy locations are correlated, [6,7].

The process to be followed here for tackling the RSDIM is that of Monte Carlo. The MC approach has been proved to be a powerful tool to study difficult problems such as random spin systems. In some cases, the simulation method suffers from problems of slow dynamics, thus, new algorithms have been proposed to overcome such difficulties. Wang–Landau (WL) [8] and entropic sampling [9] are examples of such efforts. The critical properties concern always an infinitely bulk system, since the phase transitions appear in such a system; however, from MC simulations the critical behavior is extracted from results obtained on a finite-size system by means of finite-size scaling (FSS). This process, since its inception, has been evolved as a very powerful tool for extracting properties of an infinite system near a phase transition, although it is, as yet, not fully completed causing, sometimes, ambiguities about its results. The major goal of the finite-size method is to identify the set of critical exponents that, together with other universal parameters, characterizes the universality class. As these exponents offer the most direct test of universality, their precise calculation is of great importance. However, the experimental devices are finite, consequently, the exponents cannot be measured with infinite precision causing, occasionally, controversies to distinguish the universality class a specific system belongs, [10]. For more on the theory of finite-size scaling see, e.g. Barber [11], Privman [12] and Binder [13].

For the 2D RSDIM, the nature of the possible phase transition as well as the universality class is not completely understood. The value and even the sign of the specific heat exponent α is still not known. Because of logarithmic divergence of specific heat of the pure system ($\alpha = 0$), Harris criterion is inconclusive, hence, a great deal of effort has been dedicated to elucidating the properties of the 2D RSDIM. Currently, it seems that two scenarios have prevailed, which, however, are mutually exclusive. According to the first one (*logarithmic-corrections* scenario), the critical exponents are unaffected by disorder, apart from possible logarithmic corrections (*strong-universality*), while the second, predicts critical exponents varying continuously with disorder, but the exponents' ratios (γ/ν), (β/ν) remain the same as in the pure case, *weak universality*, [4].

Kim and Patrascioiu [14] studied the 2D RSDIM on a square lattice with periodic boundary conditions and dilution-site concentration (dilution probability) $q = 1/9, 1/4, 1/3$ and lattice linear size L up to 600, using MC simulation;