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

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ABSTRACT

The influence of random bond-dilution on the critical properties of the two-dimensional Ising model on a square lattice with periodic boundary conditions is presented using the Monte Carlo process with Wang–Landau sampling. The lattice linear size is $L = 20$–140 and the concentration of the diluted bonds spans a wide range from weak to strong dilution, namely, $q = 0.05, 0.1, 0.2, 0.3, 0.4$; the respective percolation limit for the square lattice is $q_c^{PERC} = 0.5$. Its pure version ($q = 0$) has a second-order phase transition with vanishing specific heat critical exponent, an example of inapplicability of the Harris criterion. The main effort is focused on the temperature dependence of the specific heat and magnetic susceptibility to estimate the respective maximum values and subsequent pseudocritical temperatures for extracting the relative critical exponents. We have also looked at the probability distribution of the susceptibility, pseudocritical temperature and specific heat for assessing self-averaging. The study is carried out in the appropriately restricted but dominant energy subspaces. By applying the finite-size scaling analysis, the critical exponents are estimated; the specific heat exponent vanishes, the correlation-length exponent ν is equal to one and the critical exponents' ratio (γ/ν) retains its pure-Ising-model value, thus supporting the strong universality hypothesis.

1. Introduction

The critical properties of magnetic systems with quenched disorder has been the subject of growing interest in the last years, since it has been established that the introduction of randomness can cause important effects on the thermodynamic behavior of these systems in comparison to the pure ones; the type of the phase transition as well as the universality class may change [1–7]. For a second-order phase transition (SOPT) the qualitative influence of randomness is governed by Harris criterion [8]; however, for a first-order phase transition (FOPT) the situation is more complex; in two dimensions an infinitesimal amount of disorder converts it into an SOPT, whereas in three dimensions it is converted to an SOPT when disorder exceeds a threshold [4–6]. Randomness is encountered in the form of vacancies, variable or diluted bonds, impurities [9], random fields [10], etc. Its influence on the critical behavior and magnetic properties is a long-standing and still unsettled problem in statistical physics and an important question that has arisen is the extent to which randomness influences the critical behavior. In addition, the study of disordered systems is a necessity because homogeneous systems are, in general, an idealization, whereas real materials contain impurities, nonmagnetic atoms or vacancies randomly distributed within the system consisting of magnetic atoms, or variable bonds; such systems have attracted wide interest and have been studied intensively theoretically, numerically and experimentally, since it is of great importance to develop an understanding of the role of these non ideal effects. To facilitate the study, these are modelled by using pure system model modified accordingly, e.g. Ising, Potts, Baxter-Wu, etc. Such systems are the randomly dilute uniaxial antiferromagnets,

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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 non-magnetic materials. A significant contribution towards this study was proposed by Harris [8]; it relies on the pure model specific heat critical exponent α_{pure} and concerns weakly disordered systems, although the notion "weakly disordered" is not strictly clear; according to this criterion the uncorrelated weak disorder is relevant, implying that a new random fixed point governs the critical phenomena of the disordered system if α_{pure} is positive (e.g., the three-dimensional Ising model), while if α_{pure} is negative then disorder becomes irrelevant as in the three-dimensional Heisenberg model.

The pure two-dimensional (2D) Ising model (IM) constitutes a marginal situation as regards the Harris criterion since $\alpha_{pure} = 0$; consequently, it has attracted great interest for elucidating the properties of its disordered versions. By disorder it is implied either random site one [1–4,9,11–18] or bond one [1–3,7,19–24]; such a system possesses two types of fluctuations, the usual thermal as well as the disorder; both should be included in the calculations of the physical quantities in order to obtain reliable results.

A great deal of effort has been spent for the site-diluted lattices, wherein some of the sites are occupied by magnetic atoms, whereas the remaining ones are either occupied by nonmagnetic atoms or are vacant. The corresponding zero-magnetic field randomly site-diluted Ising model (RSDIM) Hamiltonian is,

$$H = -J \sum_{\langle i,j \rangle} c_i c_j S_i S_j, \quad S_i = \pm 1 \tag{1}$$

where $J > 0$ is the interaction constant, ferromagnetic interactions. The coefficients c_i's, called occupation variables, are quenched, uncorrelated random variables chosen to be equal to 1 with probability p when the i-site is occupied by a magnetic atom and 0 with probability $q = 1 - p$ otherwise; the respective probability distribution is $P(c_i) = p\delta(c_i - 1) + q\,\delta(c_i)$, bimodal probability distribution function. The summation in (1) runs over all nearest neighbor pairs of the lattice of linear size L. In a previous communication, we have examined the two-dimensional RSDIM on a square lattice with periodic boundary conditions [9]; now, we shall turn our efforts towards the study of the two-dimensional randomly bond-diluted Ising model (RBDIM), wherein some of the bonds are randomly missing, in order to study the respective critical phenomena associated with the ferromagnetic phase transitions of this model and examine whether it changes universality class or not.

The majority of publications for the bond disordered Ising model concern the case of anisotropic interactions, i.e., the exchange interaction J_{ij} is an uncorrelated quenched variable taking the values J, J', drawn from the probability distribution $P(J_{ij}) = p\delta(J_{ij} - J) + (1 - p)\delta(J_{ij} - J')$; the advantage of this choice is that the critical temperature T_c results from the duality relation $\sinh(2\beta_c J)\sinh(2\beta_c J') = 1$ for $p = 1/2$, which is the preferred choice for p [25,26]. The early Monte Carlo (MC) and renormalization group studies suggested that the critical exponents of the diluted systems are identical to those of the pure model [27–30]; however, soon after the advent of computers and the improvement of simulations, conflicting results started to appear [2,3,11–14,9,19,15–18,20–23]. Currently, it seems that two scenarios have prevailed, which, however, are mutually exclusive. According to the first approach, the critical exponents vary continuously with disorder, but the exponents' ratio (β/ν), (γ/ν) remains the same as in the pure case, *weak universality* [11–14,9,19]; the second scenario (*logarithmic-corrections* scenario) predicts that the critical exponents are unaffected by disorder, apart from possible logarithmic corrections (*strong-universality*) [2,3,15–18,20–23]. An important result of the first approach is that the specific heat critical exponent α is negative so that the specific heat approaches an asymptotic value in the thermodynamic limit [14,9]. The experimental confirmation of Harris criterion was reported in a two-dimensional order–disorder transition, wherein the values of the critical exponents (β, γ, ν) change from those of the four-state Potts universality class to Ising-like exponents close to T_c [31]. Dotsenko and Dotsenko (DD) [2], in their seminal papers, pioneered the theoretical research of diluted systems; they predicted new critical behavior for the specific heat, magnetization, correlation length and susceptibility, namely,

$$\begin{aligned}
&C_V \propto |\epsilon|^{-\alpha} \ln[1 + C \ln(1/|\epsilon|)] + C' \\
&m \propto \exp\left\{-\frac{A}{2}[\ln\ln(1/|\epsilon|)]^2\right\} \\
&\xi \propto |\epsilon|^{-1}[1 + C|\ln(1/|\epsilon|)|]^{1/2} \\
&\chi \propto |\epsilon|^{-2}\{-A[\ln\ln(1/|\epsilon|)]^2\}
\end{aligned} \tag{2}$$

where $\epsilon = (T - T_c)/T_c$, T_c the critical temperature, C, C', A are constants and $\alpha = 0$. The second and fourth expressions in (2) yield new values for the critical exponents β and γ, namely, $\beta = 0$ and $\gamma = 2$. However, Shalaev [3], Shankar [20], Ludwig [21] (SSL) questioned DD conclusions; making use of bosonization techniques and conformal invariance they corroborated DD specific heat prediction, but not that for magnetization and susceptibility, instead they concluded that,

$$\begin{aligned}
&m \propto |\epsilon|^{1/8}[1 + \lambda \ln(1/|\epsilon|)]^{-1/16} \\
&\chi \propto |\epsilon|^{-7/4}[1 + \lambda \ln(1/|\epsilon|)]^{7/8}
\end{aligned} \tag{3}$$

where λ is a smooth function of the dilution q. Although the expressions for susceptibility found by DD and SSL differ, they agree that it diverges at T_c. SSL found that magnetization and susceptibility follow power laws with the same critical exponents as the pure model, modified by logarithmic corrections, as well. Ballesteros et al. [16], Selke et al. [17] as well as Kenna et al. [18], by performing MC simulations, concluded that disorder is irrelevant; the specific heat and