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

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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 \( \alpha \), thus, the Harris criterion is inconclusive, in that disorder is a relevant or irrelevant perturbation for the critical behavior 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 \( \nu \) was found to be greater than one, whereas the ratio of the critical exponents \( (\alpha/\nu) \) is negative and \( (\gamma/\nu) \) retains its pure Ising model value supporting weak universality.

Key words: Lattice theory, two-dimensional Ising model, randomness, site dilution, Monte-Carlo, Wang-Landau, finite-size scaling
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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., \(Fe_qZ_{1-q}F_2\), \(Mn_qZ_{1-q}F_2\), \(Fe_{1-q}Al_q\), obtained by mixing uniaxial antiferromagnets with non-magnetic 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 favorite 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 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 behavior 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 behavior 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 behavior if the specific heat critical exponent \(\alpha\) 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 $\pm 1$. One can also consider a modified version of this model wherein some of the lattice sites, chosen randomly, are either vacant or occupied by non-magnetic 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 $\alpha$ 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 dis-
order, apart from possible logarithmic corrections (*strong-universality*), while the second, predicts critical exponents varying continuously with disorder, but the exponents’ ratios \((\gamma/\nu), (\beta/\nu)\) 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; their conclusions are that the specific heat does not diverge for \(q = 1/4, 1/3\) while for \(q = 1/9\) it seems to increase as \(\epsilon \to 0, \epsilon = (T - T_c)/T_c, T_c\) critical temperature. The magnetic susceptibility \(\chi\) and correlation length \(\xi\) fit the pure power law, the value of the respective exponent \(\gamma\) and \(\nu\) increases with \(q\) while \(\eta = 2 - \gamma/\nu\) remains the same as in the pure system. Queiroz and Stinchcombe [15] using transfer-matrix-scaling technique, Mazzeo and Kühn [16] following the same technique with the equilibrium ensemble approach to disordered systems, came to the same conclusions. Newman and Riedel [17], using renormalization group on weakly diluted systems confirmed the existence of a new stable fixed point with new exponents. Heuer [18] focused on the exponents \((\gamma/\nu)\) and \((\beta/\nu)\) for the 2D RSDIM on a square lattice with \(72 \leq L \leq 250\) and \(0 \leq q \leq 0.4\); according to his estimations, \((\beta/\nu)\) does not change notably with dilution within the errors and, practically, it assumes its pure system value. The exponent \((\gamma/\nu)\) shows a strong dilution-dependence in the temperature range \(10^{-2} < (T - T_c)/T_c < 1\), but near \(T_c\) it asymptotically approaches the pure system value \((7/4)\) independently of dilution.

On the other hand, Shchur and Vasilyev [4] analyzing the MC data for the magnetic susceptibility critical amplitudes \((\Gamma, \Gamma')\) above and below the critical temperature, respectively, for dilution \(q \leq 0.25\) and lattice linear size up to \(L = 256\), concluded that the ratio \((\Gamma/\Gamma')\) seems to remain constant for the dilute-site concentrations considered and equal to its pure system value. This implies that the 2D RSDIM belongs to the same universality class as the pure one. Dotsenko and Dotsenko [19], Shalaev [20], Shankar [21], Ludwig [22], using field theoretical calculations, showed that randomness is irrelevant (critical exponents are unchanged) and only logarithmic corrections might appear in the case of weak dilution; they found for the correlation length, magnetization and susceptibility, respectively,

\[
\xi \propto |\epsilon|^{-1}[1 + \lambda \ln(1/|\epsilon|)]^{1/2} \tag{1}
\]

\[
m \propto |\epsilon|^{1/8}[1 + \lambda \ln(1/|\epsilon|)]^{-1/16} \tag{2}
\]

\[
\chi \propto |\epsilon|^{-7/4}[1 + \lambda \ln(1/|\epsilon|)]^{7/8} \tag{3}
\]

while the specific heat diverges as \(\ln(\ln L)\)

\[
C_V \propto |\epsilon|^{-\alpha} \ln[1 + C \ln(1/|\epsilon|)] + C' \tag{4}
\]
where $\lambda$ is a smooth function of $q$, $\alpha = 0$ and $C'$ a constant. Ballesteros et al [23], by performing MC simulations in conjunction with finite-size scaling (FSS) for $p = 1, 8/9, 3/4, 2/3$, although observed small deviations of the values of the critical exponents from those of the pure system on varying the concentration, they considered it as a transient effect, since this can be lifted if a pure Ising value for the exponents is combined with logarithmic corrections. Selke et al [24], using MC techniques for lattices with linear size $8 \leq L \leq 256$ and spin concentration $0.1 \leq p \leq 1$, concluded that impurities lead the specific heat to diverge as $C \sim \ln(\ln L)$ on approaching the critical temperature. Tomita and Okabe [25] performed MC simulations on the same system on a square lattice using the probability-changing cluster (PCC) algorithm confirming that randomness is irrelevant and its influence is evident through logarithmic corrections.

Allowing for the previous arguments, we remark that in spite of much effort devoted to the investigation of RSDIM in the critical region, the question of the dependence of critical exponents on randomness is still open. In this paper, we shall examine the critical properties of the 2D RSDIM using an alternative approach based on the WL algorithm. In this analysis, the major goal will be to estimate the critical temperature and exponents of the 2D RSDIM for various values of the spin concentrations to assess whether it belongs to the Ising universality class or not by studying the finite-size behavior of the specific heat and magnetic susceptibility.

The paper is organized as follows. In the next section, after the introduction of the model, we shall discuss the approach based on the WL algorithm and an efficient implementation by conveniently restricting the simulation in the dominant energy subspace. In section 3 we apply the FSS to the Ising model under consideration and we close with the conclusions and discussions in section 4.

2 Numerical approach of the RSDIM

We consider the Hamiltonian of the two-dimensional site-diluted Ising model, in the absence of any external field,

$$H = -J \sum_{<ij>} c_i c_j S_i S_j, \quad S_i = \pm 1, \quad (5)$$

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; that is, we have the probability distribution $P(c_i) = p \delta(c_i - 1) + q \delta(c_i)$. The summation extends over all nearest-neighbor pairs of the square lattice, of linear size $L$ with periodic boundary conditions.
The data was generated by extensive MC calculations using WL sampling method to estimate the density of states (DOS) \( g(E) \) [8]. WL sampling performs a random walk with an acceptance ratio \( P(E_i \rightarrow E_j) = \min\{1, \frac{g(E_i)}{g(E_j)}\} \), where \( E_i \) and \( E_j \) are the energies before and after the transition, respectively, aiming at sampling a flat histogram in energy. The WL algorithm overcomes the difficulties, such as critical slowing down and long relaxation times in systems with complex energy landscape, appearing in other MC processes. This algorithm has been applied to a wide range of systems spanning from the Ising model [26,27], random field Ising model [28], 3D conserved-order-parameter Ising model [29], Potts [30], to glassy systems [31], polymers [32], DNA [33] and the Baxter-Wu model [34]. The DOS \( g(E) \) is not constant during the random walk, it is modified according to the rule \( g(E) \rightarrow (g(E) \cdot f) \); the modification factor \( f \) varies as \( f_{j+1} = \sqrt{f_j} \), \( j \) is the order of iteration. In the current investigation, the WL algorithm performed 26 iterations and the initial value for \( f \) was \( f = e \).

Having an accurate estimation of \( g(E) \), the non-normalized canonical distribution can be constructed, \( P(E,T) = g(E) e^{-\beta E} \); subsequently, the partition function can be calculated through the expression \( Z(T) = \sum_E g(E) e^{-\beta E} \), from which most of the thermodynamic observables can be estimated. This kind of MC simulation constitutes a major improvement towards speeding calculations since it avoids multiple runs (one for each temperature) needed by the majority of MC algorithms to describe the temperature dependence of thermodynamic quantities over a significant temperature range; in a WL algorithm temperature is not needed to be specified a priori. In the present case, the WL algorithm was implemented on lattices with \( 20 \leq L \leq 120 \) and the density of states was stored as a function of the energy. The dilution \( q \) can vary from 0.0 (\( p = 1 \)) to the percolation threshold \( q_{PERC}^{PERC} = 0.407255 \) (\( p_c^{PERC} = 0.592745(2) \)), [35].

The quantities, upon which we shall rely for studying the critical behavior of the RSDIM, are the specific heat \( C = \frac{\langle E^2 \rangle \rangle - \langle E \rangle^2}{(NT)^2} \) and magnetic susceptibility \( \chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{(NT)} \), per particle. The MC data is generated by choosing a realization of the dilution for a specific value of \( q \) and various values of \( L \). This procedure is then repeated for several other realizations for a specific value for the lattice linear size \( L \). For each realization, we find the maximum value of the specific heat \( (C^*(q,L)) \) and susceptibility \( (\chi^*(q,L)) \), recording simultaneously the values of the respective pseudocritical temperatures, \( T^*_c(q,L) \) and \( T^*_\chi(q,L) \), respectively, forming in each case, a sequence of “pseudocritical temperatures” converging to the critical temperature \( T_c(q) \) of the infinite system as \( L \rightarrow \infty \). Among the different realizations large fluctuations are observed in the same set of the previous quantities.

The presence of randomness is evident in the way averaging processes are
carried out for an observable $X$, which assumes a different value for each of the $M$ random realizations of the disorder corresponding to the same value of dilution $q$. This implies that $X$ behaves as a stochastic variable, whose mean value is estimated through a two-step process. First, the usual thermal average is performed for a specific realization of the dilution. After the completion of the $M$ realizations of randomness, the disorder average is carried out over the $M$ realizations and is denoted by the brackets $[\cdot]$.

For the 2D IM the specific heat and magnetic susceptibility in the thermodynamic limit diverge; in a finite lattice, this divergence is rounded off and manifests itself by a maximum exhibited by the above quantities. This maximum increases gradually with $L$ and ultimately tends to infinity as $L \to \infty$. For the 2D RSDIM, in attempting to detect the maximum $C^*(q, L)$ of the specific heat and the respective temperature $T^*(q, L)$ (pseudocritical temperature), we considered two routes. Let $C_m(q, L)$ be the specific heat for a particular realization $m$ out of $M$ realizations for a specific dilution $q$. In the first route, we estimated, initially, the maximum value $C^*_m(q, L)$ together with the respective pseudocritical temperature $T^*_C(q, L)$ for every realization $m$ of the disorder; then, we considered the sample average of the individual specific heat maximum $[C^*(q, L)]$ and pseudocritical temperature $[T^*_C(q, L)]$, for the $M$ realizations,

$$[C^*(q, L)] = \frac{1}{M} \sum_{m=1}^{M} C^*_m(q, L), \quad [T^*_C(q, L)] = \frac{1}{M} \sum_{m=1}^{M} T^*_C(q, L)$$  \hspace{1cm} (6)$$

In the second route, following Rieger and Young, the sample summation for the specific heat for the totality of $M$ realizations was considered [36],

$$[C(q, L)]_{sum} = \frac{1}{M} \sum_{m=1}^{M} C_m(q, L)$$  \hspace{1cm} (7)$$

In (7), the resulting specific heat curve is very complex with many local maxima, reflecting the strong pseudocritical temperature fluctuations in the ensemble of random realizations. From these maxima we selected the absolute one, indicated by $[C(q, L)]_{sum}^{*} = max[C(q, L)]_{sum}$, occurring at the pseudocritical temperature $T^*_{C, sum}(q, L)$. The same procedure was also followed for the magnetic susceptibility $\chi$; the resulting quantities are denoted by $[\chi^*(q, L)]$, $[T^*_\chi(q, L)]$, $[\chi(q, L)]_{sum}$, $T^*_{\chi, sum}(q, L)$.

To investigate the critical behavior of the system, we performed extensive MC simulations to calculate the density of states $g(E)$ for each value of dilution $q$ and $L$ through the WL algorithm. After estimating the density of states $g(E)$, one can proceed to the calculation of the necessary thermodynamic quantities, such as the energy $E$, specific heat $C_L(T)$, magnetization $M$ and susceptibil-
ity $\chi_L(T)$ for further use in order to identify the probable universality class. However, before proceeding to this end, we outline a new restricted method for speeding up the numerical calculations; this method is called “Critical Minimum Energy Subspace” (CrMES) technique, [27,29,34]. In this method, we concentrate our simulation only on the dominant energy subspaces. In the following lines we describe its implementation. Consider the specific heat per site for a lattice of linear size $L$ at temperature $T$,

$$C_L(T) = L^{-d}T^{-2} \left\{ Z^{-1} \sum_{E_{\min}}^{E_{\max}} E^2 \exp[S(E) - \beta E] - \left( Z^{-1} \sum_{E_{\min}}^{E_{\max}} E \exp[S(E) - \beta E] \right)^2 \right\}$$  \hspace{1cm} (8)$$

where the Boltzmann constant was set $k_B = 1$, thus $\beta = 1/T$, $d$ is the spatial dimension ($d = 2$) and $Z$ the “partition function” of the system,

$$Z = \sum_{E_{\min}}^{E_{\max}} \exp[S(E) - \beta E]$$  \hspace{1cm} (9)$$

The latter expression is the partition function in case $g(E)$ is the exact DOS of the system and properly normalized, [37]. In practice, the DOS, resulting from WL simulations, is an approximate result whose accuracy depends on that of the simulation. In the expression (8), the calculation of the specific heat in the critical region can be speeded up by restricting the energy interval if we use the CrMES technique. Let $\tilde{E}$ be the energy corresponding to the maximum term $\exp[S(E) - \beta E]$ of the partition function (9) for the temperature at hand. Because of the sharpness of the energy distribution, the energy interval $(E_{\min}, E_{\max})$ in the summation (8) is replaced by a smaller one $(\tilde{E}_{-}, \tilde{E}_{+})$ around $\tilde{E}$ corresponding to a predefined accuracy $r$ for the specific heat expressed as, $| [C_L(\tilde{E}_{-}, \tilde{E}_{+})/C_L(E_{\min}, E_{\max})] - 1 | \leq r$, where $r = 1 \cdot 10^{-6}$ and $\tilde{E}_{\pm} = \tilde{E} \pm \Delta_{\pm}$, $\Delta_{\pm} \geq 0$. The induced errors are much smaller than the ones in determining the DOS, for more see [27]. The magnetic properties were obtained using the final stages of the WL algorithm, following our earlier proposal as in [38].

3 Finite-size scaling analysis. Results

The FSS is based on the assumption that the free energy of a system of linear size $L$ and in the absence of an external magnetic field scales as,

$$F(L, \epsilon) = L^{-\psi}F_0(\epsilon L^\theta)$$  \hspace{1cm} (10)$$

where $\psi = (2 - \alpha)/\nu$. The scaling of the correlation length $\xi = \xi_0 \epsilon^{-\nu}$ suggests
that $\theta = \nu^{-1}$. The scaling function $F_0(x)$ is universal, in that, it is independent of the lattice size.

Fig. 1. Specific heat finite size approximations against $\ln L$ (squares) and $\ln \ln L$ (circles) for $q = 0.3$.

The quantity that specifies the scenario the RSDIM shall follow is, nevertheless, the specific heat. According to the $\ln \ln L$ scenario the specific heat diverges as in (4), while according to weak universality and FSS, the specific heat obeys the power law,

$$[C^*(q, L)] = p_1 + q_1 L^{\alpha/\nu}$$

In this expression the lack of the correction terms speeds up the convergence and yields more stable fits.

The choice of the suitable asymptotic law for the specific heat has caused considerable concern, since one has to choose between Eqs. (4) and (11); thus, we have checked both. In the pure two-dimensional Ising model, $q = 0$, the specific heat against $\ln L$ is a straight line, representing the forthcoming divergence, while against $\ln \ln L$ the respective curve bends upwards, see Fig. 6 in [16] as well as Ref. [39]. Plotting the specific heat data for $q = 0.3$ against $\ln L$ and $\ln \ln L$, respectively, see Fig. 1, we observed that the former curve (rightmost in Fig. 1) bends downwards deviating from a straight line, whereas the latter curve (leftmost) seems to bend also downwards implying that the data does not follow the $\ln \ln L$ scenario. The same behavior was also observed for
Table 1
The critical temperature and critical exponents resulting from the sample average of the specific heat (6) and the respective expression for susceptibility, for different values of spin dilution \( q \). For each \( q \)-value, the first line corresponds to the specific heat data and the second to the susceptibility.

| \( q \) | \( T_c \) | \( \nu \) | \( \alpha/\nu \) | \( C^\infty \) | \( \gamma/\nu \) |
|--------|------|------|--------|---------|--------|
| 0.1    | 1.90668(0.00101) | 1.152090.036990.03476 | -0.26406(0.02552) | 2.38683(0.09096) | 1.74968(0.01369) |
|        | 1.90271(0.00219) | 1.151810.038130.03576 |                 |                  |
| 0.2    | 1.50675(0.00137) | 1.182090.026470.02534 | -0.30892(0.01719) | 1.24453(0.01400) | 1.74918(0.00983) |
|        | 1.50180(0.00342) | 1.182890.047760.04419 |                 |                  |
| 0.3    | 1.15280(0.00385) | 1.236290.057590.05251 | -0.38223(0.03119) | 0.71851(0.00659) | 1.74939(0.01643) |
|        | 1.10051(0.00211) | 1.237180.029490.02815 |                 |                  |

the dilution \( q = 0.2 \), but this is more evident for the stronger dilution \( q = 0.3 \); for \( q = 0.1 \) it is not so evident because this is a crossover case.

Mazzeo and Kühn ([16]) checking the credibility of both scenarios, studied initially the lnlnL one; by fitting their data to this law, they concluded that it was difficult to accept definitely this scenario (4); instead, they focused on the power law (11) and estimated the \( \alpha \)-exponent for various dilutions, testing the validity of the respective values by using the hyperscaling relation in combination with the \( \nu \)-exponent, estimated earlier. Their data resulted from calculations on the equilibrium ensemble approach together with numerical transfer matrix technique, phenomenological renormalization group scheme and conformal invariance on finite-width strips.

In addition, we have also invoked the \( \chi^2 \)-test to discriminate between Eqs. (4) and (11) by estimating the ratio between the \( \chi^2 \)-test for the lnlnL scenario with the one for the power law suggested by (11): for \( q = 0.2 \) this ratio is 2 while for \( q = 0.3 \) it is 3, indicating an increasing tendency with \( q \); hence, although the above description makes evident the need for data on much larger systems sizes, we shall adopt the power law (11) as it seems to be more suitable and reliable for the present case. This practice shall be followed in the sequel.

Firstly, we fit the specific heat sample average maxima to the power law (11). Considering a specific value for \( q \) and extrapolating towards \( L \to \infty \) the respective values of \( [C^\ast(q, L)] \), one can read off the asymptotic value \( p_1 \equiv C^\infty \) as well as the critical exponents ratio \( (\alpha/\nu) \); these appear in Table 1 for the dilutions \( q = 0.1, 0.2, 0.3 \). We have also considered that the maximum values \( [C(q, L)]_{\text{sum}}^\ast \) of the specific heat resulting form sample summation, see (7), follow a similar power law as in (11), but with different symbols for the respective quantities,
Table 2
The critical temperature and critical exponents resulting from the sample summation for the specific heat (7) and the respective expression for susceptibility, for different values of spin dilution $q$. For each $q$-value, the first line corresponds to the specific heat data and the second to the susceptibility.

| $q$ | $T_c$     | $\nu$  | $\alpha/\nu$ | $C^\infty$  | $\gamma/\nu$ |
|-----|-----------|--------|---------------|--------------|--------------|
| 0.1 | 1.89557(0.00218) | 1.15335(0.06633) | $-0.26412(0.02986)$ | 2.29555(0.0988) |
|     | 1.90329(0.00322) | 1.15303(0.05880) | 1.74934(0.00694) |
| 0.2 | 1.49638(0.00272) | 1.18318(0.04952) | $-0.30877(0.01983)$ | 1.18223(0.01361) |
|     | 1.50281(0.00387) | 1.18293(0.05486) | 1.74931(0.00963) |
| 0.3 | 1.08592(0.00621) | 1.23752(0.06445) | $-0.38221(0.03831)$ | 0.53077(0.00704) |
|     | 1.07301(0.00426) | 1.23634(0.05141) | 1.74925(0.02756) |

Fig. 2. Specific heat fitting according to the FSS prediction (11). The specific heat corresponds to the sample average (6) and site dilution $q = 0.1$. For $q = 0.2, 0.3$ the plots are similar. The coefficients $P_1, P_2, P_3$ correspond to $p_1, q_1, \alpha/\nu_C$, respectively, see Eq. (11).

$$[C(q, L)]_{\text{sum}} = \bar{p}_1 + \bar{q}_1 L^{\bar{\alpha}/\bar{\nu}_C}$$

(12)

Fitting the respective values to (12) and extrapolating towards $L \longrightarrow \infty$, the values for $\bar{p}_1$ and $(\bar{\alpha}/\bar{\nu}_C)$ are estimated and appear in Table 2 for the same $q$ values. In both Tables, the asymptotic values of the specific heat form two decreasing sequences as $q$ increases and it seems that they tend to zero at the percolation threshold ($q_c = 0.407255$); the non-divergence is also evident by the levelling off of the specific heat data, indicative of approaching a saturation value, see Fig 2; the specific heat follows a similar behavior for the other
two values of \( q \), as well. The main outcome of this fit is that the exponents’ ratio \((\alpha/\nu)\) appears to be negative, exhibiting a steady decreasing tendency approaching the percolation value \( \alpha/\nu = -0.5 \), [40].

For any value of \( q \), the respective critical temperature \( T_c \) is not known a priori (as it happens to be for the random bond counterpart [41]) although there exists a formula \( T_c(q) = T_c(0)(1 - 1.565q) \), \( T_c(0) \) is the pure system critical temperature [42], but of limited applicability since it is valid only for small impurity concentrations, thus the estimation of the \( T_c \) for any \( q \) is of great importance. The correlation length exponent \( \nu \) is directly related to the specific heat exponent \( \alpha \) through the hyperscaling relation \( \alpha + d\nu = 2 \) (\( d \) system’s dimensionality, \( d = 2 \)) which acts as a constraint; the nondivergence of the specific heat \((\alpha < 0)\) is consistent with \( \nu > 1 \) for the current model. Assuming the FSS prediction,

\[
\begin{align*}
[T_C^*(q, L)] &= T_{c,C} + b_1 L^{-1/\nu_C} \\
[T_\chi^*(q, L)] &= T_{c,\chi} + c_1 L^{-1/\nu_\chi}
\end{align*}
\]

(13)

Fig. 3. Specific heat pseudocritical temperature fitting according to the first equation of the FSS prediction (13). The sequence corresponds to the sample average (6) and site dilution \( q = 0.1 \). For \( q = 0.2, 0.3 \) the plots are similar. The coefficients \( P_1, P_2, P_3 \) correspond to \( T_{c,C}, b_1, (1/\nu_C) \), respectively, see Eq. (13).

one can estimate the critical temperatures \( T_{c,C} \) and \( T_{c,\chi} \) resulting from the sample averages of the specific heat and susceptibility, respectively, as well as the corresponding exponent \( \nu \), see Fig. 3. Also, similar scaling laws are con-
Fig. 4. Susceptibility fitting according to the first equation of the FSS prediction (15). The specific heat corresponds to the sample average and site dilution \( q = 0.1 \). For \( q = 0.2, 0.3 \) the plots are similar. The coefficients \( P_1, P_2, P_3 \) correspond to \( r_0, s_1, (\gamma/\nu_\chi) \), respectively, see Eq. (15).

Considered for respective quantities for the sample summation but with different symbols for the involved quantities, see [36],

\[
\begin{align*}
T_{c,\text{sum}}^*(q, L) &= \tilde{T}_{c,C} + \tilde{b}_1 L^{-1/\nu_C} \\
T_{\chi,\text{sum}}^*(q, L) &= \tilde{T}_{c,\chi} + \tilde{c}_1 L^{-1/\nu_\chi}
\end{align*}
\]

Fitting the respective pseudocritical temperatures for both routes of the specific heat and susceptibility to (13) and (14), they yield the values of the critical temperature and \( \nu \) exponent appearing in Tables 1, 2. In both Tables, the respective values for \( \nu \) vary continuously with dilution \( q \) and are greater than one in conformity with hyperscaling. It seems that the critical temperature decreases to zero as the dilution \( q \) increases towards the percolation limit \( q_c = 0.407255 \). For the low impurity concentration, \( q = 0.1 \), the deviations of the respective values of the critical temperature is small, as well as for the intermediate \( q = 0.2 \), see Tables 1, 2. For \( q = 0.1 \), the average of the four values is \( \langle T_c(q = 0.1) \rangle = 1.9020625 \), which agrees with that in Heuer [18] (1.9004427), Tomita and Okabe [25] (1.9022), Shchur and Vasilyev [4] (1.9032), and consistent with that from the formula in Ref. [42], \( T_c(q = 0.1) = 1.9141 \). For the intermediate impurity concentration \( q = 0.2 \), the average of the respective critical temperatures is \( \langle T_c(q = 0.2) \rangle = 1.5016825 \); it is in agreement with that in Heuer [18] (1.507873), Shchur and Vasilyev [4] (1.5103), while deviates from that of the formula in Ref. [42], \( T_c(q = 0.2) = 1.558930 \). For the large impurity concentration \( q = 0.3 \), the first value of critical temperature in Table 1
(1.15280) shows significant deviation from the other three, so if we consider only the remaining three their mean value is \( T_c(q = 0.3) = 1.08648 \), consistent with that in Heuer [18] (1.075140), and Tomita and Okabe [25] (1.0712), while disagrees with that in Ref. [42] \( T_c(q = 0.3) = 1.10306 \).

We have also considered the FSS for both susceptibility averages. The maximum values \( [\chi^*(q, L)] \) and \( [\chi(q, L)]_{\text{sum}}^{*} \) for both routes follow the scaling laws,

\[
[\chi^*(q, L)] = r_0 + s_1 L^{\gamma/\nu_x} \\
[\chi(q, L)]_{\text{sum}}^* = \tilde{r}_0 + \tilde{s}_1 L^{\tilde{\gamma}/\tilde{\nu}_x}
\]  

(15)

In (15), we have considered that both background terms vanish \( (r_0 = \tilde{r}_0 = 0) \), since this gives more stable fits. Fitting the respective numerical data for both routes of susceptibility to (15), the ratio \( (\gamma/\nu) \) was estimated and their values appear in Tables 1, 2 for the same dilutions, see Fig. 4. In both Tables, the ratio \( (\gamma/\nu) \) retains its pure Ising model value \( (\gamma/\nu = 7/4) \) independently of dilution, thus corroborating the weak universality hypothesis.

Fig. 5. Probability distribution of the relative susceptibility vs relative susceptibility \( \chi_r (\chi_r = \chi_j/\langle \chi \rangle, \chi_j, \langle \chi \rangle \) are the j-bin and global average susceptibility, respectively) for dilutions \( q = 0.1(a), 0.3(b) \) and lattice linear size \( L = 30, 70, 90 \). The non-self-averaging behavior is evident from the persistence of the width of the plots as the lattice linear size \( L \) increases.

An important issue arising in a disordered system is the notion of self-averaging, that is, to what extent properties of the system depend on the particular realization of the quenched random variables, implying that the distribution of an observable becomes sharper as \( L \) increases. In case their relative widths remain constant as \( L \to \infty \), then we say the system is non-self-averaging, [43]. In the pure Ising model the respective distributions transform into delta functions as \( L \to \infty \). To investigate the possibility of such a behavior in the current disordered model, we produce \( N_s \) samples of an observable \( X \) (e.g.,
specific heat, susceptibility) and form the respective probability density distribution \( P(X_j/\langle X \rangle) \), where \( X_j \) and \( \langle X \rangle \) are the value of the observable in the \( j \)-bin and its global average, respectively. If we identify \( X \) with system’s susceptibility \( \chi \), then the resulting probability density \( P(\chi_i/\langle \chi \rangle) \) as a function of \( (\chi_i/\langle \chi \rangle) \) for \( q = 0.1, 0.3 \) and \( L = 30, 70, 90 \) appears in Fig. 5. The respective curves of the relative susceptibility for a specific value of dilution collapse on each other irrespective of the value for \( L \) and they do not become sharper on increasing \( L \). The general shape of the curves remains the same independently of the value for \( q \). This behavior implies non-self-averaging. Similar behavior was also displayed by the respective plots of pseudocritical temperatures and heat capacity.

4 Conclusions and discussions

We have presented MC numerical data on the 2D RSDIM for three cases of dilution spanning a wide range of dilution, \( q = 0.1, 0.2, 0.3 \), i.e., weak, intermediate and strong, for lattices with linear size in the range \([20, 120]\), using FSS and following the Wang-Landau algorithm for the calculation of the density of states. The calculations dealt with the estimation of the critical temperature, the critical exponent \( \nu \) and ratios \( (\alpha/\nu) \) and \( (\gamma/\nu) \). The results indicate that as \( q \) increases \( \nu \) increases, while \( (\gamma/\nu) \) remains constant and \( (\alpha/\nu) \) decreases. A consequence of the invariance of \( (\gamma/\nu) \) is that the exponent \( \eta = 2-(\gamma/\nu) \) is invariant, as well. Using the Rushbrooke equality \( \alpha + 2\beta + \gamma = 2 \) in conjunction with hyperscaling relation \( \alpha + d\nu = 2 \), we deduced that \( (\beta/\nu) \) is also invariant, retaining its pure Ising value, \( \beta/\nu = 1/8 \). Referring to the critical temperature, although there exist four different sequences, resulting from the various procedures for any dilution \( q \), each one exhibits a decreasing tendency, tending to zero as \( q \) tends to the percolation limit \( q_c = 0.407255 \).

A notable feature of the current-model data is the asymptotic behavior of the specific heat as \( L \) increases; it tends to a saturation value for any \( q \), in contradistinction to its counterpart in the pure model that diverges. The other critical quantity, susceptibility, still diverges as \( L \to \infty \).

An important issue is that if impurity concentrations larger than \( q = 0.3 \) towards the percolation limit \( q_c \) are considered, then the high dilution shall reduce significantly the long-range correlations enhancing in this way the finite-size effects; to moderate this effect larger lattices are needed at the cost of larger computer-execution time.

Our results and findings are supporting the argument that the 2D RSDIM does not belong to the same universality class as the pure 2D Ising model but to a new one. In conclusion, the present results favor the weak universality scenario.
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