Specific heat of two–dimensional diluted magnets

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Abstract

Using Monte Carlo techniques, the two–dimensional site–diluted Ising model is studied. In particular, properties of the specific heat, its critical behaviour and the emergence of a non–singular maximum above the transition temperature at moderate concentration of defects, are discussed.

Key words: Two–dimensional Ising model, site–dilution, specific heat, Monte Carlo simulations

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1. Introduction

The effect of randomness on the critical properties of two–dimensional Ising magnets has attracted much interest. [1–3] Based on field–theoretical renormalization group calculations, it has been argued that weak randomness will modify the critical behaviour of the perfect case marginally. For instance, the specific heat $C$ is found to diverge on approach to the critical temperature, $T_c$, in a doubly logarithmic form [1,2]

$$C \propto \ln(\ln t) \quad (1)$$

where $t = |T - T_c| / T_c$ is the reduced temperature. In the pure case, $C$ displays the well–known logarithmic singularity.

Results of numerical studies, using Monte Carlo methods and finite–size transfer matrix techniques, on the two–dimensional bond–diluted Ising model, even at moderate or rather strong dilution, are in accordance with the field–theoretical
predictions [4–10], albeit some of the data leave room for alternate interpretations.–

Attention may be also drawn to related recent simulations on two–dimensional Potts and Ashkin–Teller models. [11,12]

On the other hand, simulations on the two–dimensional site–diluted Ising model seemed to indicate that the critical peak in $C$, present at weak dilution, disappears at moderate dilution, well below the percolation threshold [13], with a broad maximum above the critical temperature. [14–18] Certainly, a finite value of the specific heat at $T_c$ would invalidate (1). However, recent Monte Carlo work [19] suggests that the field–theoretical results may be correct also in the case of moderate site–dilution. Indeed, $C(T_c)$ is found to increase with the linear size, $L$, of the system like $\ln(\ln L)$. Accordingly, quite large system sizes might be required to monitor a peak in $C$ near $T_c$.

In any event, a careful and systematic investigation on the emergence of the non–critical broad maximum in the specific heat and on the fate of the critical peak in $C$ with increasing dilution is much needed. In this paper, we shall present results of such a study.

2. Model, method and results

We consider a square lattice with sites $i$. A randomly chosen fraction $1 – p$ of the sites are assumed to be occupied by Ising spins, $S_i = \pm 1$, coupled by ferromagnetic nearest–neighbour interactions, $J$. The remaining fraction, $p$, of sites is ‘empty’ (or occupied by non–magnetic ions). Accordingly, $p = 0$ refers to the perfect case. The transition temperature $T_c(p)$ is lowered by increasing the concentration of defects, $p$. It vanishes at and above the percolation threshold, $p_c \approx 0.40725$ [13,20], see Fig. 1.

The simulations were done using the Wolff cluster–flip algorithm and, for small lattices or at temperatures well above $T_c$, the Metropolis single–spin–flip method. We considered quadratic lattices of $L \times L$ sites with full periodic boundary conditions; $L$ ranging from 8 to 256. The dilution $p$ varied in between 0 and 0.9. Apart from the energy, $E$, and the specific heat per spin (which we computed both from the energy fluctuations and the temperature derivative of the energy), $C$, we recorded the absolute value of the magnetization $|m|$ and the susceptibility, $\chi$ (as well as other quantities related to properties of the Wolff clusters [21]). We monitored the behaviour of single realizations of the site–randomness and of ensembles of $N$ realizations (with $N$ going up to 1000). For each realization, we averaged over up to $10^7$ clusters (or up to several $10^6$ Monte Carlo steps per site), after equilibration.
Fig. 1. Phase diagram of the two–dimensional site diluted Ising model with the transition line $T_c$ and the location of the non–critical maximum $T_m$ of the specific heat, as obtained in previous and the present simulations.

To set the frame for the following discussion, the phase diagram is depicted in Fig. 1, based on previous large–scale simulations [17–19], which we checked and augmented. The phase transition line, $T_c(p)$, is observed to decrease almost linearly with dilution up to about $p \approx 0.3$, and then it bends over to vanish at the percolation threshold, i.e. $T_c(p_c) = 0$. In addition, the location of the non–critical maximum in the specific heat, $T_m(p)$, is shown in Fig. 1 (its location does not depend strongly on system size, see below).

For illustration, examples of the temperature dependence of the specific heat, $C(T)$, at various concentrations of defects $p$, are shown in Fig. 2, with linear dimension $L = 64$, for single realizations of the site–dilution. At weak randomness, one observes a pronounced peak around the critical temperature, with the height decreasing rapidly with increasing dilution. At moderate dilution ($p = 0.26$, in the figure), the specific heat displays at temperatures above $T_c$ a shoulder, eventually turning over into the non-critical maximum, at $T_m(p)$, which persists at defect concentrations above the percolation threshold up to arbitrarily large dilution. The height of the non–critical maximum decreases only mildly for stronger dilution.

The region of moderate dilution, say, $0.25 < p < 0.35$, deserves special attention, in order to, possibly, disentangle the critical peak in $C$ from the non–critical maximum above $T_c$. In particular, the kind of the realization, i.e. of the distribution of the spins on the lattice, and the system size are important.
Fig. 2. Specific heat, $C$, versus temperature, $k_B T/J$, for single realizations with $L=64$ at various concentrations of defects, $p=0.15, 0.26, 0.3, 0.55, \text{ and } 0.7$; see also Fig. 1.

We did an extensive study of this region by considering mostly $p=0.26, 0.30, \text{ and } 0.35$, monitoring a wide range of realizations and lattice sizes.

Note that very good statistics is needed to establish unambiguously especially the subtle features in the shape of $C$ in that region. The accuracy of the data has been checked, for instance, by looking for consistency in the averages for $C$ as obtained from the temperature derivative and from the fluctuations of the energy. Eventually, we took into account up to $10^7$ clusters, close to $T_c$, or several $10^6$ Monte Carlo steps per site, using the Wolff or Metropolis algorithm. We checked and confirmed, that our results are independent of the type of the simulative algorithm (the two methods are complementary, with the Wolff algorithm being more powerful at low temperatures and close to criticality for large systems). We also used different random number generators to avoid possible dangerous correlations arising from an unfortunate choice of that generator [22] (indeed, for the dilute model, both linear congruential and shift register random number generators are suitable). Note that previous simulative results, when based on significantly shorter Monte Carlo runs, should be viewed with much care.

Fig. 3 summarizes our findings on the specific heat $C$ at $p=0.3$, with $L$ ranging from 8 to 256, where the number of maximal realizations $N$ for the various lattices is decreasing from 1000 to 4. The statistical errors for each realization are very small. However, deviations between different samples, fixing the number of sites and spins, may be large, especially for small lattices (say, up to $L=64$; at $L=64$, some of the single realizations still show only the broad
maximum above $T_c$, while others exhibit an additional, albeit weak, peak at $T_c$). Therefore, the total bars stem mostly from the ensemble averaging. By adjusting the number of samples, $N$, to the size of the lattice, $L$, the resulting errors were always smaller than the size of the symbols in Fig. 3. As seen from that figure, the non–critical maximum in $C$ and the peak close to $T_c$ can be easily discriminated by simulating sufficiently large systems (which had not been noted before). The shape of the non-critical maximum becomes independent of the lattice size for sufficiently large systems. It may be interesting to note that the appearance of a rather narrow peak at $T_c$ had been suggested before by one of us [23], discussing possible similarities to analytic findings on other random models [24]. Doing standard finite–size analyses [25], we estimated the critical temperature $T_c$ from the location of the turning point in $|m|$ and from the critical peak in $C$ to be $k_B T/J = 1.084 \pm 0.001$ (being slightly higher than a previous estimate [17]). We found the shift of the deviation of the location of the anomalies from $T_c$ to be nearly proportional to $1/L$ for sufficiently large $L (\geq 64)$. The specific heat at $T_c$ for finite lattices, $C(T_c, L)$, was then obtained by interpolation between close–by data of $C(T)$, leading to increased error bars.

As depicted in Fig. 4a, $C(T_c, L)$ seems to approach, for $L \geq 32$, a doubly logarithmic form, $C = C_0 ln(ln L) + C_1$, in accordance with the field–theoretical prediction for weak randomness. The prefactor $C_0$ is quite small, $C_0 \approx 0.17$ (with $C_1 \approx 0.27$), similarly to findings in the bond–diluted case for moderate dilution. [4] Consistently, $C(T_c, L)$ seems to increase more slowly than logarithmically for sufficiently large lattices, while a logarithmic increase is
Fig. 4. Specific heat $C$ vs. lattice size $L$, using a doubly logarithmic (a) and a logarithmic (b) scale for $L$, at the estimated critical temperature $k_B T_c = 1.084J$ for $p = 0.30$. Lines are guides to the eye.

conceivable for smaller lattices, see Figs. 4a and 4b. The crossover to the dilution dominated critical regime may be described by casting $C(T_c, L)$ in the form $C = C_0 \ln(b + \ln L) + C_1$, as had been obtained before for the bond–diluted Ising model. [4] We confirmed that the plots are insensitive towards the exact determination of $T_c$, accepting the accuracy of our estimate ($k_B T_c/J = 1.084 \pm 0.001$). Of course, the situation in the bond–diluted Ising model, where $T_c$ is known exactly, is more convenient. [4]

At $p = 0.26, one observes a broad shoulder in $C$ above $T_c$, which one may associate with the non–critical maximum, superimposed and masked by critical fluctuations. At $p = 0.35$, the specific heat displays a broad maximum well above $T_c$, compare to Figs. 1 and 2. Around $T_c$ (estimated from $\chi$ and
In a microscopic description, the neighbouring lattice sites occupied by spins form distinct clusters. Certainly, spins in different clusters do not interact with each other, and thermodynamic quantities are obtained by summing over the contributions of separate clusters. For instance, the specific heat may be written as \( C = \sum C_k \), summing over all clusters, \( k \).

At \( p < p_c \), in the thermodynamic limit \( L \to \infty \), there exists one cluster with infinitely many spins covering a non-zero fraction of the lattice sites. That cluster, corresponding to the largest cluster in finite systems, is expected to carry the critical properties, and the other remaining clusters do not lead to non-analytic thermal averages. Of course, the weight of the contributions of the remaining clusters to the non-singular features of many thermal quantities is expected to grow as the dilution increases. It may be therefore tempting to attribute the non-critical maximum in \( C \) to those clusters. However, this argument is not correct.

In particular, for defect concentrations \( p \) of about 0.3, we determined the contributions to \( C \) due to the largest and the other clusters separately. We found that the energy fluctuations of the other clusters are far too small to account for the shoulder and the non-critical maximum in \( C \) above \( T_c \). Actually, most of the finite clusters consist of single spins, with vanishing specific heat. On the other hand, the largest cluster has a rather ramified structure. There are many weakly connected subclusters of various sizes, which may act essentially like separate clusters. [13] Those subclusters may flip completely near \( T_c \), with a small change of energy resulting from the spins at the links between them. Accordingly, the contributions of such excitations to the specific heat (i.e. the temperature derivative of the energy) may be still small. These excitations, however, affect strongly the magnetization and its fluctuations, i.e. the susceptibility, leading to pronounced peaks in \( d|m|/dt \) and in \( \chi \) near \( T_c \). Presumably most importantly, the number of perimeter spins, i.e. spins with neighbouring empty sites, is quite large [13], reflecting the loose structure of the largest cluster. The perimeter spins, which have a reduced coordination number, are thermally excitable at a characteristic temperature, leading to near-by local disordering and a pronounced change in energy in that temperature region. Therefore, they may contribute significantly to the shoulder and, upon further dilution, to the non-critical maximum (note that this feature is valid and specific for site-dilution. Indeed, for bond-diluted Ising models, \( C \) shows no
anomalies above the critical point [26]). The critical behaviour of $C$, in turn, is expected to be due to the rather compact backbone of the largest cluster [13]. The size of the backbone scales with the lattice size, $L^2$, at $p < p_c$, and it may eventually give rise to a divergent peak in $C$.

Increasing the dilution, with $0.3 < p < p_c$, a growing number of spins will no longer belong to the largest cluster, which, itself, will become even more ramified. As a result the non–critical energy fluctuations will be enhanced, and the, supposedly, critical contributions of the compact backbone of the largest cluster become more and more suppressed, requiring larger and larger system sizes to detect the possibly singular critical behaviour of $C$.

At $p > p_c$, in the thermodynamic limit, there is no cluster of spins covering a non–zero fraction of the lattice (the largest cluster is believed to grow with system size like $\ln L$ [13], while the number of lattice sites increases with $L^2$). As a consequence, e.g., the infinite cluster cannot stabilize the ordered phase at non-zero temperatures, and $T_c(p) = 0$. Obviously, the remaining finite clusters contribute more significantly to, e.g., the specific heat at stronger dilution. Their average size shrinks with rising dilution, leading to the shift of the broad maximum in $C$ towards lower temperatures, $T_m$. Actually, the smallest temperature would be reached if there would be predominantly clusters consisting of one or two spins. The maximum of $C$ for clusters of two spins is readily calculated to be $T_m = 0.8335...J/k_B$. Indeed, this temperature seems to be approached when $p \longrightarrow 1$, see Fig.1.

3. Summary

Using Monte Carlo techniques, the specific heat $C$ of the site–diluted two–dimensional Ising model has been studied as a function of temperature, lattice size, and degree of dilution, considering single realizations of the dilution as well as ensembles of samples.

Upon increasing the dilution, we observe the systematic evolution of a non–critical maximum above the critical point. In turn, eventually, rather large system sizes are then needed to detect the narrow critical peak at $T_c$. Indeed, we showed unambiguously the existence of the corresponding two–maxima structure in $C$ at moderate dilution, $p = 0.3$, for lattices with linear dimension $L \geq 128$. That aspect had not been noted before. The critical behaviour of the peak at $T_c$ seems to be, at $p = 0.3$, in accordance with the field–theoretical predictions. In particular, the Monte Carlo data are compatible with a crossover, for sufficiently large lattices, to the dilution dominated regime where $C(T_c, L)$
increases in a doubly logarithmic form with $L$.

A microscopic picture, based on the geometric aspects of the clusters of spins (perimeter and backbone spins of the largest cluster, weakly coupled subclusters and separate small clusters), is proposed allowing to describe qualitatively, and partly even quantitatively, the properties of the specific heat observed in the simulations.

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