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The critical region of the random-bond Ising model

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Abstract. We describe results of the cluster algorithm *special purpose processor* simulations of the 2D Ising model with impurity bonds. We use large lattices with up to 10^6 spins to define critical temperature regions where both finite-size corrections and corrections to scaling are small. High-accuracy data unambiguously show an increase in the magnetization and magnetic susceptibility effective exponents β and γ, caused by impurities. The M- and χ-singularities become sharper, while the specific heat singularity is smoothed.

1. Introduction

The problem of the influence of inhomogenities on phase transitions has a long history. The first model with some kind of impurity to be studied is, due to its simplicity, the Ising model. The effect of randomness on the critical behaviour of different Ising models has been investigated by Harris [1]. He found that if the specific heat of the pure system diverges as some power of $(T_c - T)^{-1}$, then the critical behaviour will be changed by impurities. Such a result does not give any information for the 2D Ising model, which has a logarithmic divergence of the specific heat.

Theoretical treatment of the 2D Ising model with ferromagnetic impurity bonds was pioneered by Dotsenko and Dotsenko (DD) [2–6]. They predicted new critical behaviour of the specific heat [2, 3], spin–spin correlation function, magnetization and magnetic susceptibility [4, 5]. Later the same model was considered in a number of theoretical studies [7–15]. Some authors claimed the specific heat should be finite for all temperatures [14, 13]. Others [7–12] (SSL) confirmed the DD result for the specific heat, but stated the critical behaviour of spin–spin correlation function and magnetization to be the same, or almost the same, as in the pure case, only slightly changed by logarithmic corrections.

Experiments on quasi-2D compounds with almost Ising spins [16–20] did not show any deviations from Onsager results, probably because of the insufficient accuracy caused by large-scale inhomogeneities which smooth out the phase transition. Moreover, in such experiments it is not possible to exclude 3D effects. Hence, to understand whether any of the theories contain essential physics, it is necessary to perform computer simulations.

Early Monte Carlo simulations [21, 22] demonstrated the same critical behaviour as in the pure case.

The large-scale simulations were started by Andreichenko *et al* [23–25]. The specific heat at the critical point of the model with impurities $C(T_c)$ was studied as a function of the system size L [24, 25]. For large impurity strengths the specific heat $C(T_c)$ was found to be proportional to $\log\log(L)$, which seems to be in agreement with the DD prediction.

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The behaviours of the magnetization $M(T_c)$ and magnetic susceptibility $\chi(T_c)$ as functions of L turned out [24, 25] to be the same as in the pure case, which contradicted the DD theory.

Usually, critical behaviour is studied as a function of relative temperature distance $\tau = (T_c - T)/T_c$ from T_c. Some deviations from the pure behaviour of $M(\tau)$ and $\chi(\tau)$ were found by Wang *et al* [25], and in *special purpose processor* (SPP) simulations [26, 27]. The accuracy of [25–27] was not, however very high, and the critical region was not defined.

The new SPP simulation [28, 29], using the cluster Wolff algorithm, allows a very accurate description of the 2D random Ising model critical behaviour. It gives us not only the thermodynamic quantities, but also the spin–spin correlation function [29, 30]: $\mathrm{CF}(r) = \langle S(0)S(r)\rangle$ which has been directly studied theoretically [4–12].

2. The model

We study the same system as was considered earlier [23–27]. Ising spins are located at the nodes of a two-dimensional square lattice. To avoid the appearance of border-induced terms, we use periodic boundary conditions in both directions.

Disorder is introduced via random distribution of impurity coupling constants over lattice bonds. The pure case exchange interaction constant is denoted by J, and the impurity coupling constant by J'. The probability of finding J' on some bond is p,

and the probability of finding J is $(1-p)$. In this paper we do not consider spin glasses, so both J and J' are ferromagnetic.

What can be said about the phase diagram of such a model? At $p = 0$ there is the Onsager phase transition at $(1/T_c) \approx 0.44068$, if the pure coupling constant J is chosen to be equal to 1. The shift of T_c due to impurities for small p was calculated exactly in [1, 31] for $J' = 0$, and in [3] for the general case.

Certainly, impurities destroy thermal fluctuations and decrease T_c. If there are enough strong impurities, then the phase transition disappears. Indeed, if $J' = 0$, and $p > 0.5$, then there is no percolation of bound spins in the system [32]. The lattice is broken into finite islands of interacting spins, and in a finite system there can be no phase transition.

Fortunately, for $p = 0.5$ and $J' > 0$ there exists an exact duality relation [33, 34], which gives the value of T_c as a function of J and J':

$$\tanh(J/T_c) = \exp(-2J'/T_c)\,. \tag{1}$$

In [23, 25] it was checked that the position of the specific heat maximum does indeed tend to this T_c in the limit $L \to \infty$. This confirms that there is only one phase transition point in the system.

In their theory of the impure Ising model, DD [6] introduced a small parameter g, which becomes zero if either $p = 0$ or $J = J'$. They also defined the impurity-induced length l_i as $\log(l_i) \propto 1/g$. The influence of impurities should be important only on distances larger than l_i. If the disorder is small ($g \ll 1$) then for the finite lattice with linear size L, it may happen that $l_i \gg L$. In this case it is impossible to observe the influence of impurities on the critical behaviour.

For this reason, we must choose g as large as possible to decrease l_i, in order to study the deviations caused by inhomogeneities. So, in real MC simulations g cannot be very small, and the exact theoretical formula for g given by DD [6] is no longer valid. Nevertheless, as we show later, the DD formula for the specific heat

$$C(T) \propto (1/g)\log(1 + g\log(1/\tau)) \tag{2}$$

(where g is regarded just as a parameter) describes the simulation data reasonably well .

3. Simulation procedure

We used the first cluster algorithm SPP [28, 29] for the simulations. It implements in hardware a very efficient cluster Wolff algorithm [35–37], which is an improved version of the Swendsen–Wang algorithm [38]. The Wolff algorithm does not slow down so badly at the critical point, where it should be about L^2 times faster than the conventional spin-flip algorithm. In the case of our SPP L can be as large as 1024. Thus, the improvement in speed is about one million times. A detailed description of the SPP structure and functioning can be found in [29]. The class of problems which can be solved by the SPP, is described in [28, 29].

The precise meaning of the absence of the critical slowing down was found in the simulations of the pure case [29]: the relaxation time, measured in real simulation time, is the same at the critical point as it is far from it.

The relaxation time is defined in the following way: we start simulation with all spins pointing in one direction. After some time all the thermodynamic values, such as magnetization or the lattice energy, come into the zone of thermal fluctuations near thermal equilibrium. We call this time the relaxation time.

For the pure case it is necessary to flip about 20 Wolff clusters to get to the fluctuation region near T_c, and about 5 Wolff clusters far from T_c for $L = 1024$ [29]. On the other hand, the mean number of spins in the cluster far from the critical point is almost equal to the total number of spins L^2, and near T_c the number of spins in the cluster is about four times lower. So the relaxation time, measured as the actual computer processing time, is the same.

The situation in the disordered system can be seen on figures 1 and 2. All results are given for the case where $J = 1$, $J' = 0.25$, $p = 0.5$. According to (1) this corresponds to $(1/T_c) = 0.807\,051\,86$.

Figure 1 shows the relaxation of the magnetization and the correlation function CF$(L/2)$ near T_c, for $(1/T_c) = 0.808$. We see that again, as in the pure case, 20 clusters should be flipped to enter the thermal fluctuation zone near T_c. As can be seen from figure 1, there is some correlation between M and CF$(L/2)$. Indeed, there are two ways to define M. First, we can count the difference in the number of up $(N_\uparrow)$ and down $(N_\downarrow)$ spins in the system; then the magnetization is given by

$$M_1 = (N_\uparrow - N_\downarrow)/(N_\uparrow + N_\downarrow).$$

The second definition of M is usually used obtained by finding it theoretically for the infinite system:

$$M = (\langle S(0)S(\infty)\rangle)^{1/2}.$$

In the finite system we can alternatively define M as

$$M_2 = (\mathrm{CF}(L/2))^{1/2}.$$

Our simulations show that M_1 and M_2, averaged over impurity distribution, normally lead to the same mean values of magnetization. Noticeable differences between them appear only very close to T_c, when the finite-lattice size effects come into play. Nevertheless, the correlation between M and CF$(L/2)$ persists up to T_c, as can be seen from figure 1.

The relaxation time is about 20 clusters not only for M, but also for other thermodynamic quantities. This can be seen in figure 2, which describes the relaxation of the neighbour spins correlation function CF(1). In the pure case CF(1) coincides with the energy per bond. Now it does not, because the energy is given by

$$\langle J_{01}S(0)S(1)\rangle$$

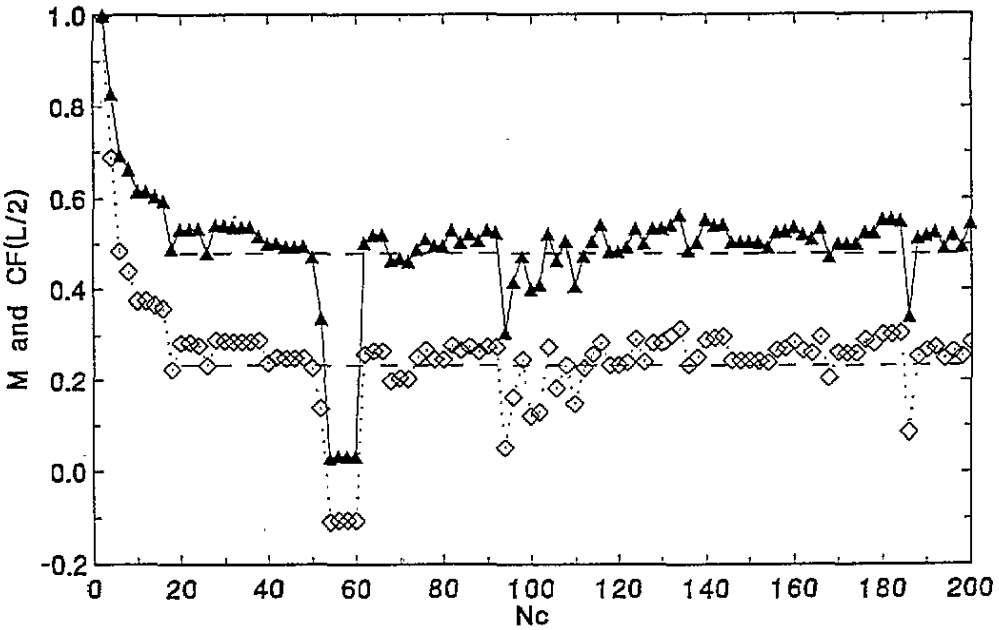

Figure 1. Time relaxation of the magnetization M (solid triangles) and of the correlation function $\mathrm{CF}(L/2)$ (empty triangles) as a function of a number N_c of flipped Wolff clusters. Broken lines show mean values, obtained for a large number of flipped clusters for the linear lattice size $L = 1024$. Temperature T is very close to T_c.

and there are some correlations between the value of the coupling constant J_{01} on the bond connecting two neighbour nodes 0 and 1, and the sign of the two-spin product. Nevertheless, the relaxation curve for the energy, also shown in figure 2, behaves very much like relaxation curve for CF(1).

Fluctuations of the magnetization, shown in figure 1, are very large, as should be the fluctuations of the order parameter near the critical point. On the other hand, the energy, which is not the order parameter, does not fluctuate so strongly. Because the relaxation time near T_c in the impure case is the same as in the pure case, we again come to the conclusion that the critical slowing down is absent. Nevertheless, to obtain the thermodynamic data described below, we permitted the spins of each sample to relax during the first 2000 cluster flips. Only after that were measurements for each sample started.

Each sample has its own distribution of impurity bonds. Coupling strengths $J = 1$ and $J' = 0.25$ were assigned to each bond with a probability one half to obey the self-duality condition. It is the difference between different samples which determines the value of standard errors for all the thermodynamic data.

We use three sets of data: low-accuracy data (obtained with 10 samples) describe the large τ-region: better data, obtained with 100 samples, give a general picture for all temperatures; finally, very accurate 1000-sample data were obtained in the critical region, where the asymptotics can be defined.

The importance of the proper determination of the critical region can be seen from figures 3 and 4, in which we show the reduced magnetization and magnetic susceptibility for the pure case, $L = 1024$ [29]. In the pure case the critical behaviour is described by the power laws

$$M_0 = 1.222\,41\,(\tau)^{1/8} \tag{3}$$

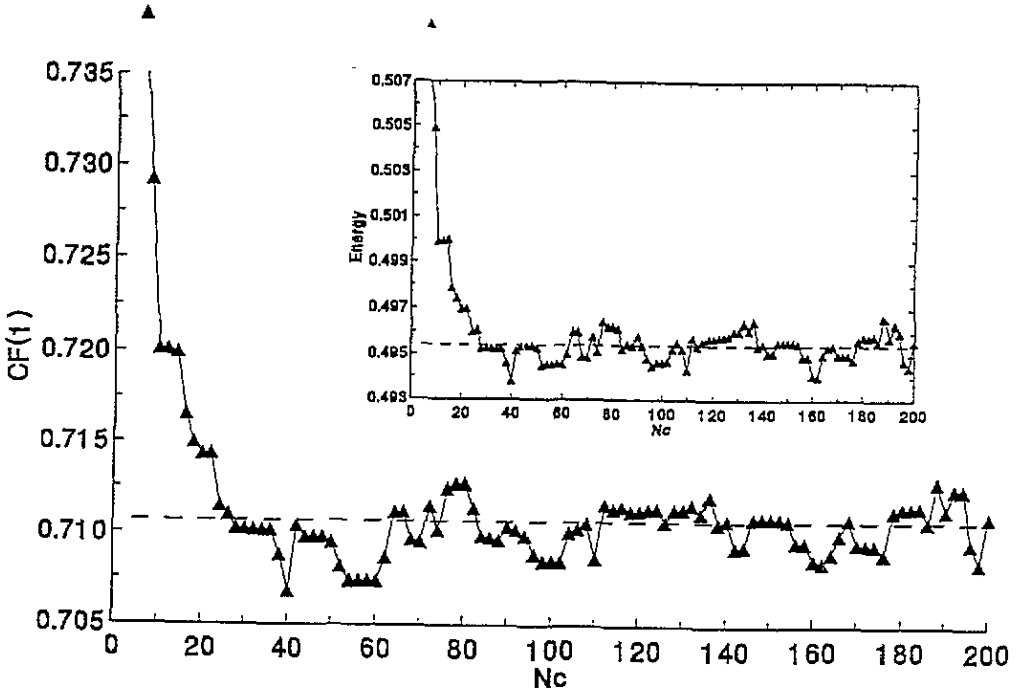

Figure 2. Time relaxation of the neighbour spin–spin correlation function CF(1) and of the energy per bond (inset). Broken lines have the same meaning as in figure 1.

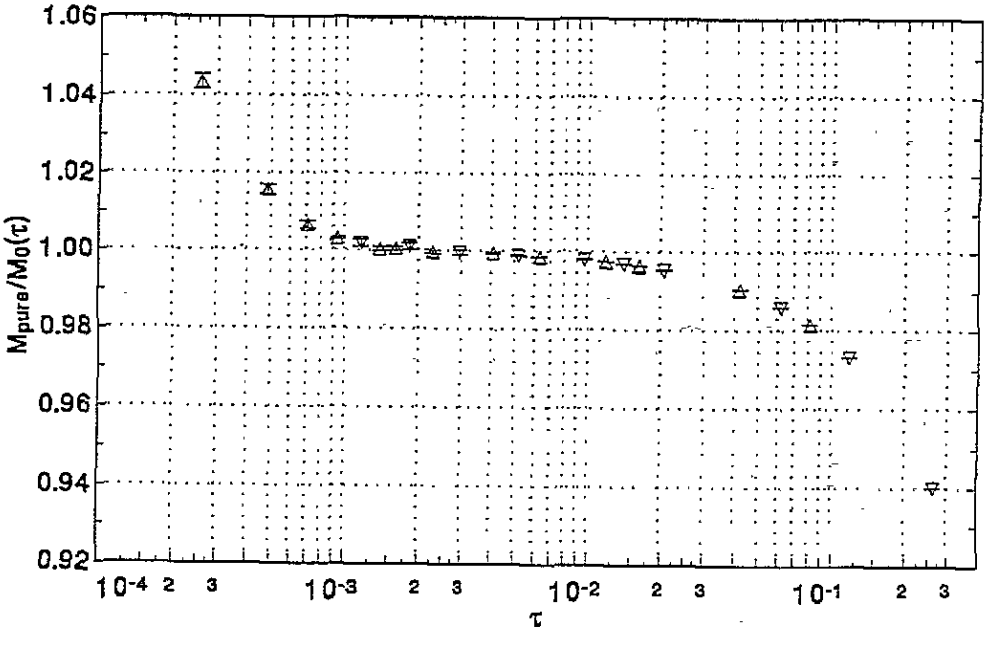

Figure 3. The ratio of the magnetization M, obtained by the cluster SPF simulation [29] for the pure Ising model, $L = 1024$, to the asymptotic law $M_0(\tau)$.

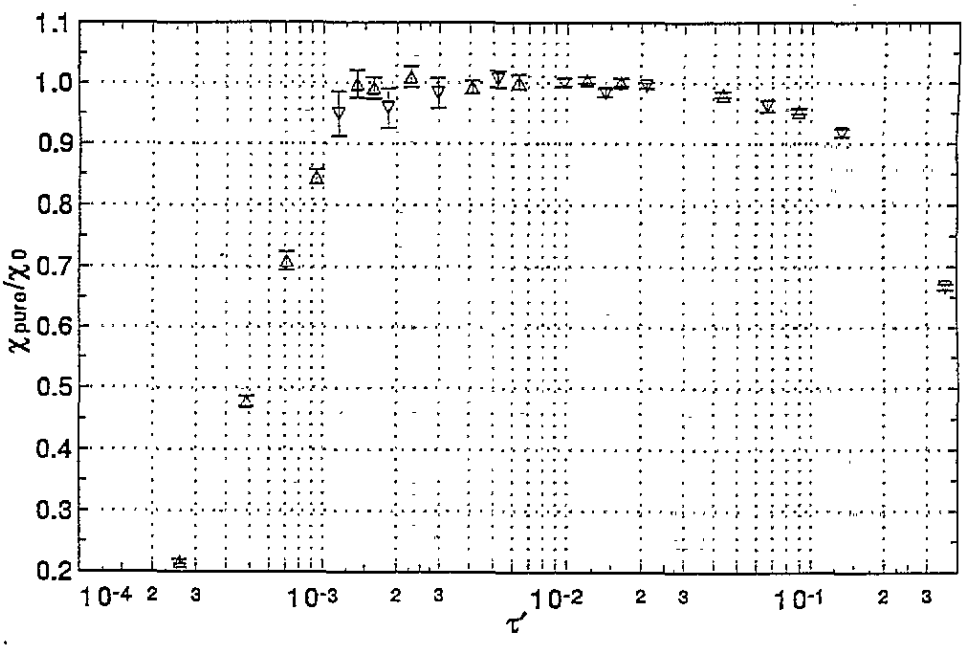

Figure 4. The ratio of the magnetic susceptibility χ, obtained by the cluster SPP simulation [29] for the pure Ising model, $L = 1024$, to the asymptotic law $\chi_0(\tau')$.

$$\chi_0 = (0.025537 - 0.001989\,\tau')\,(\tau')^{-7/4}/T \tag{4}$$

where $\tau' = (T_c - T)/T$ [39]. Figures 3 and 4 show ratios of the pure case [29] M and χ to the values obtained from asymptotic laws. It is clear that the critical region, in which the asymptotics are valid, is not very wide:

$$0.001 < \tau < 0.02. \tag{5}$$

Low-τ restriction arises from finite-lattice effects, which become important for

$$\tau < (1/L)\,. \tag{6}$$

On the other hand, we know the exact solution for the magnetization of the infinite system:

$$M_\infty = (1 - 1/\sinh^4(2/T))^{1/8}\,.$$

This solution is correct at large τ, and shows that there should be analytic corrections to the simple scaling law (3). These corrections to scaling lead to the large-τ limit in (5).

4. Results

In the impure case the asymptotics (3), (4) are no longer valid. Nevertheless, deviations from them are not very large. To see these deviations more clearly, it is convenient to again divide M and χ by M_0 and χ_0. The corresponding ratios are shown as a function of τ in figures 5 and 6. From these figures it is obvious that the critical behaviour is changed, and can be described by larger effective exponents than in the pure case. It is also obvious that the critical region for the impure case is somewhere within the range

$$0.003 < \tau < 0.03\,. \tag{7}$$

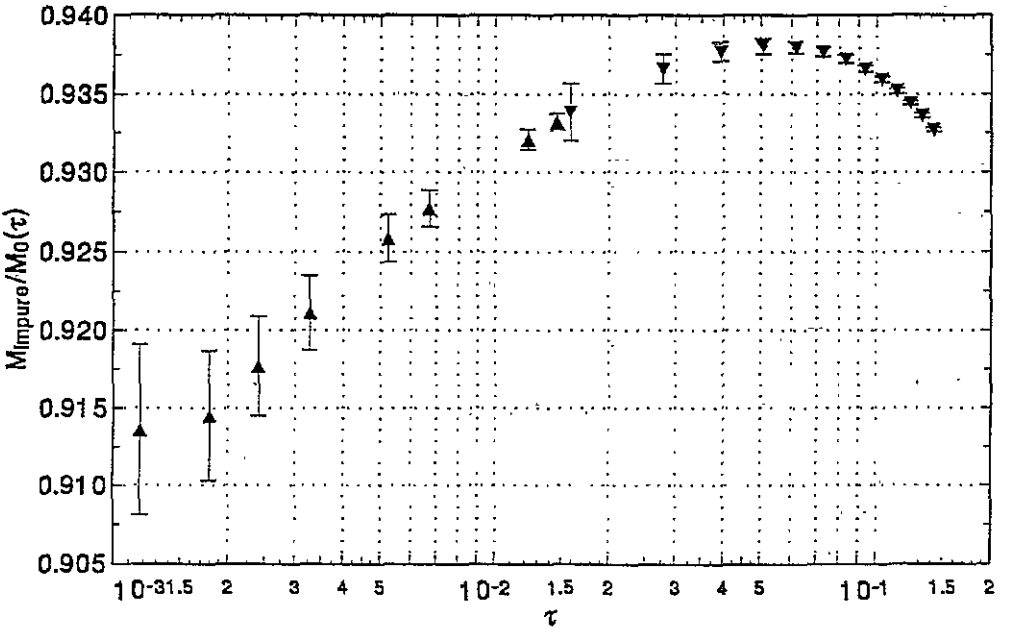

Figure 5. The ratio of the random-bond Ising model magnetization to the pure case asymptotic law $M_0(\tau)$. Down triangles show 10-sample data; up triangles show 100-sample data.

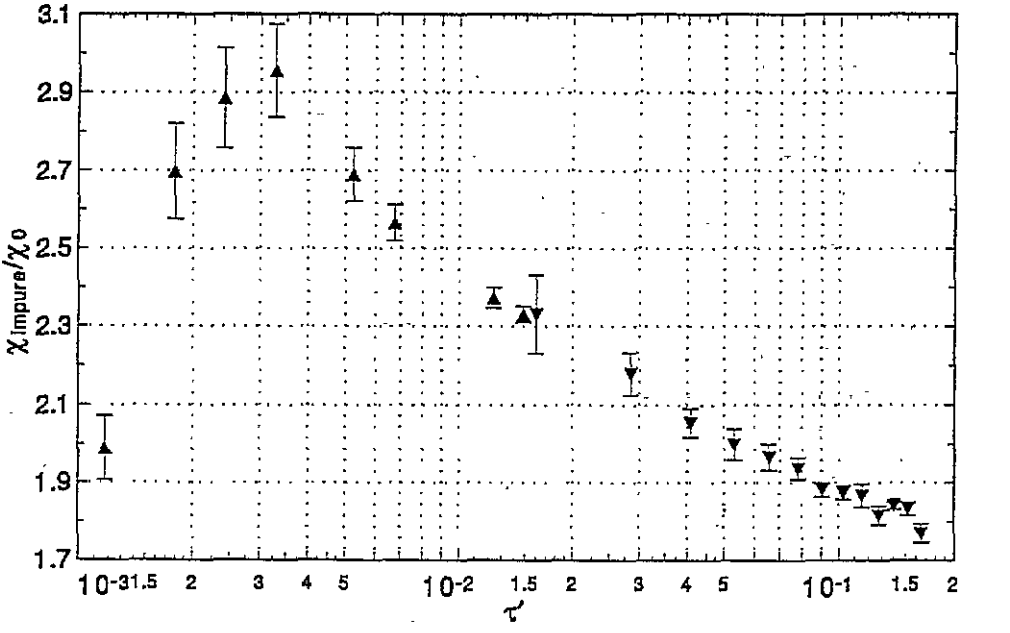

Figure 6. The ratio of the random-bond Ising model magnetic susceptibility to the pure case asymptotic law $\chi_0(\tau')$. Down triangles show 10-sample data; up triangles show 100-sample data.

To check once more that the small-τ behaviour is determined by the finite-lattice size, we show the change of this behaviour with L in figures 7 and 8. From figure 8 we see that the maximum of χ is shifted from $\tau = 0.003$ for $L = 1024$ to $\tau = 0.006$ for $L = 512$, as can be expected. It is natural to investigate the critical region (7) more carefully. The M- and χ-results obtained in this region using 1000 samples for $L = 1024$ are shown in figures 9, 10. Figure 9 shows the ratio of magnetization to (3), additionally divided by τ^{ϵ}, for $\epsilon = 0.009, 0.0075, 0.006$. We see that the effective exponent of M in the critical region is increased by 0.0075 from the pure Ising value 0.125. Figure 10 shows the analogous data for the magnetic susceptibility χ. In this case $\epsilon = -0.11, -0.135, -0.17$. This implies that the effective critical exponent for χ is $1.75 + 0.135$. These results for $M(\tau)$ and $\chi(\tau)$ definitely contradict DD [4, 5] theory.

The competing SSL theory claims that the magnetization and magnetic susceptibility retain a pure Ising dependence on the correlation length $\xi(\tau)$:

$$M_{\mathrm{SSL}}(\tau) \propto \xi^{-1/8} \qquad \chi_{\mathrm{SSL}}(\tau) \propto \xi^{7/4} \tag{8}$$

where $\xi(\tau)$ is given by the DD [2] expression

$$\xi(\tau) = \frac{1}{(1 + g\log(1/\tau))^{1/2}}. \tag{9}$$

In the absence of analytic corrections to the asymptotic laws (8), (9), our simulation data are incompatible with these laws for any value of g. On the other hand, the data agree with the following expressions:

$$M \propto (1 + a_M\tau)M_{SSL} \qquad \chi \propto (1 + a_\chi\tau)M_{SSL} \tag{10}$$

with properly chosen coefficients a_M and a_χ. These coefficients describe analytic corrections to the scaling laws, the importance of which was stressed in [25]. The value of g which should be used in (8), (9) agrees with the value of g found from the specific heat ($C(\tau)$) data, and with results given in [25].

The specific heat $C(\tau)$ is more difficult to study than the magnetization for two reasons.

(1) The specific heat is obtained as fluctuations of the energy according to the formula

$$C = \langle (E - \langle E \rangle)^2 \rangle / T^2 .$$

As a result, fluctuations of $C(\tau)$ for a given τ do not decrease with increasing lattice size L like the fluctuations of M. In reality, standard deviations of $C(\tau)$ depend only on τ and the number of flipped clusters, which was used to measure $C(\tau)$, but not on L.

(2) The specific heat τ-dependence is complicated. This creates difficulties in defining the critical region.

Figure 11 describes the general behaviour of the specific heat in both pure and impure cases as a function of τ. We see that impurities reduce $C(\tau)$ and cause deviations from the simple $\log(\tau)$ asymptotic behaviour. It is convenient to study the difference between $C(\tau)$ and its supposed asymptotics. The number of samples is equal to 100 in both cases. Only the τ-dependence or τ-independence of y is important, so all the differences in figures 11–14 are displaced by arbitrary constants.

The pure case asymptotic of $C(\tau)$ per node for $\tau \to 0$ is

$$C_0^{\mathrm{pure}}(\tau) = 0.4945\log(1/\tau) \tag{11}$$

plus some constant. Analytic 'corrections to scaling' can be made visible, if we draw the difference, $y_{\mathrm{pure}}(\tau)$, between the exact solution for the infinite lattice $C_{\mathrm{exact}}^{\mathrm{pure}}(\tau)$ and (11). This difference

$$y_{\mathrm{pure}}(\tau) = C_{\mathrm{exact}}^{\mathrm{pure}}(\tau) - 0.4945\log(1/\tau) + 0.6 \tag{12}$$

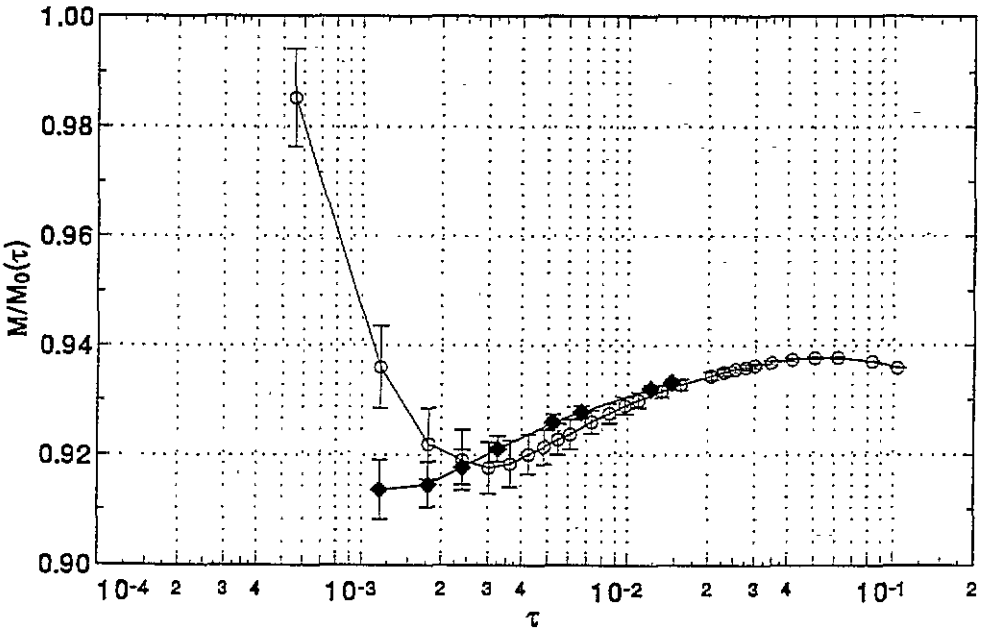

Figure 7. The impure case $M(\tau)/M_0(\tau)$ for two different lattice sizes. Empty circles show $L = 512$ data; solid diamonds show $L = 1024$ data.

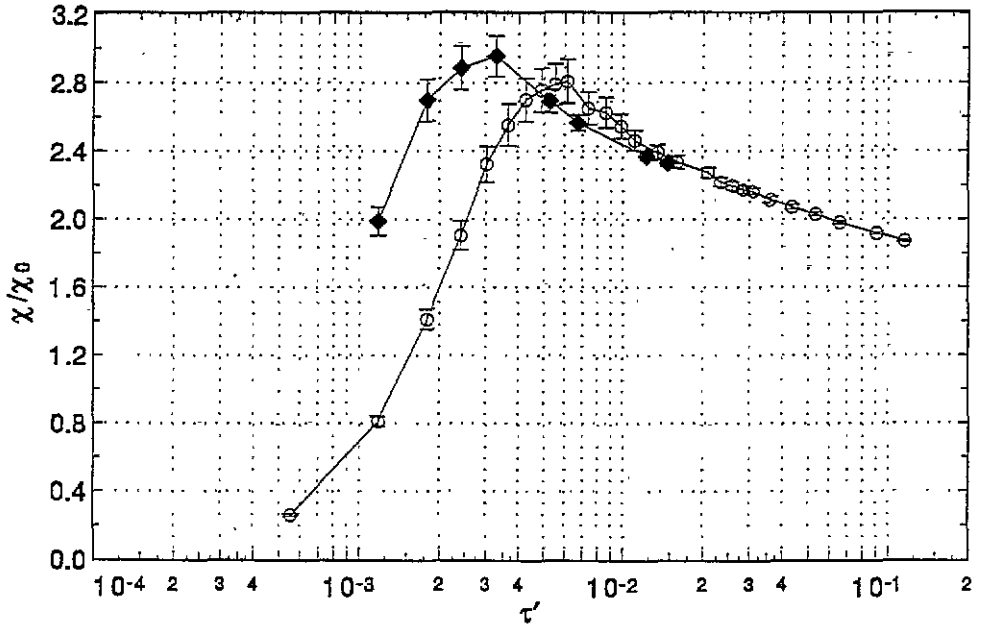

Figure 8. Impure case $\chi(\tau')/\chi_0(\tau')$ for $L = 512$ (empty circles) and $L = 1024$ (solid diamonds).

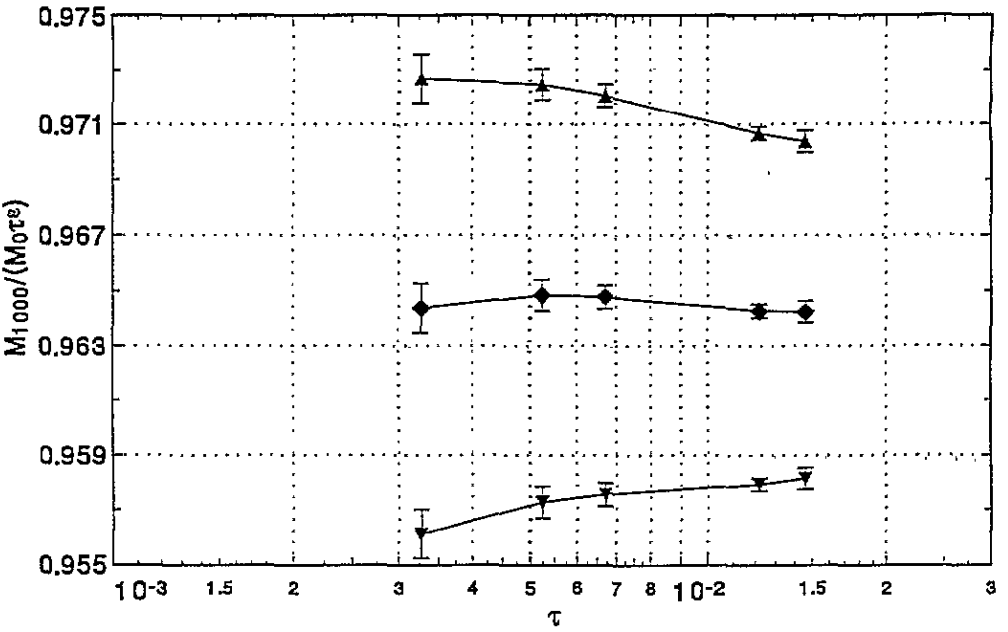

Figure 9. 1000-sample critical region magnetization data for the impure case, $L = 1024$. $M/(M_0\tau^{\epsilon})$ for $\epsilon = 0.006$ (down triangles), 0.0075 (diamonds), 0.009 (up triangles).

is shown in figure 12. Small deviations from the horizontal at large τ demonstrate 'corrections to scaling' for the simple logarithmic behaviour of $C^{\text{pure}}_{\text{exact}}(\tau)$.

The data for the impure case in figure 12 are described by the curve

$$y(\tau) = C(\tau) - 0.21\log(1/\tau). \tag{13}$$

The coefficient 0.21 before $\log(\tau)$ in this formula was chosen to make the $y(\tau)$-curve horizontal near $\tau = 0.01$. We see that deviations from the pure logarithmic behaviour are larger in the impure case. For this reason we may try to approximate $C(\tau)$ by (2). It is natural to try to choose the proportionality coefficient in such a way that for $g \to 0$ this formula becomes the pure Ising formula. Then $C(\tau)$ must be chosen as

$$C(\tau) = \frac{0.4945}{g}\log(1 + g\log(1/\tau)) + \text{constant} \tag{14}$$

where g and the constant are parameters to be found from comparison with the simulation data.

Figure 13 shows

$$z(\tau) = C(\tau) - \frac{0.4945}{0.295}\log(1 + 0.295\log(1/\tau)) + 0.6. \tag{15}$$

Here $g = 0.295$ was chosen to make the curve as close to horizontal as possible in the critical region $\tau > 0.003$. Comparison with the pure case curve on the same figure, figure 13 shows that 'corrections to scaling' for the DD formula (14) are of approximately the same value as in the pure case. The choice of $g = 0.295$ is justified by figure 14, which shows 1000-sample data for $L = 1024$ in the critical region. Figure 14 gives the curves $z(\tau)$ for three different values of g : 0.31, 0.295, 0.28. We see that the DD formula (14) describes the impure case specific heat reasonably well .

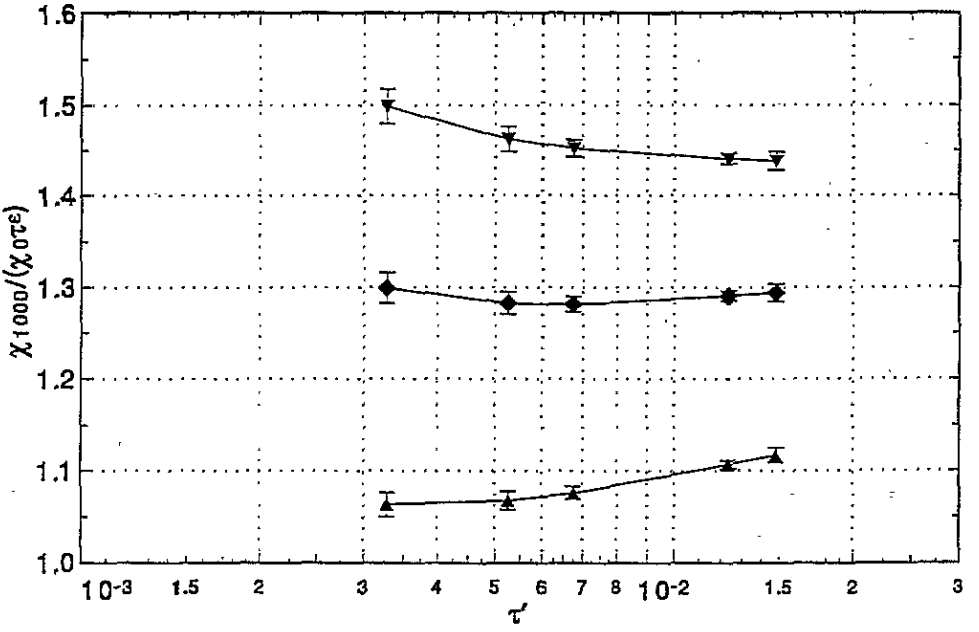

Figure 10. 1000-sample critical region χ-data for the impure case, $L = 1024$. $\chi/(\chi_0(\tau')^\epsilon)$ for $\epsilon = -0.11$ (down triangles), -0.135 (diamonds), -0.17 (up triangles).

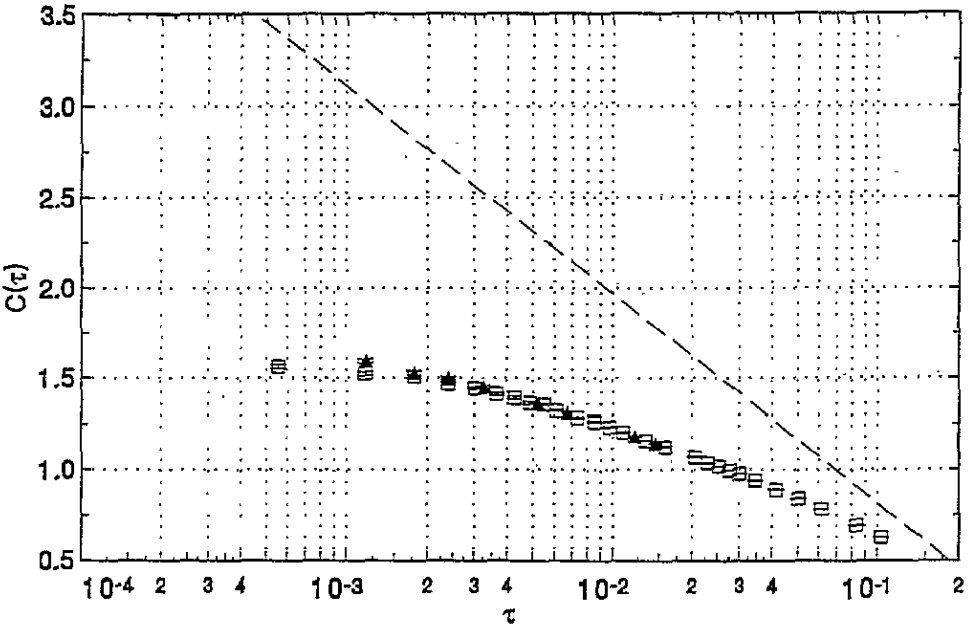

Figure 11. The specific heat per node $C(\tau)$ for the $L = 1024$ impure system (up triangles), $L = 512$ impure system (empty boxes), and infinite pure Ising system (broken line).

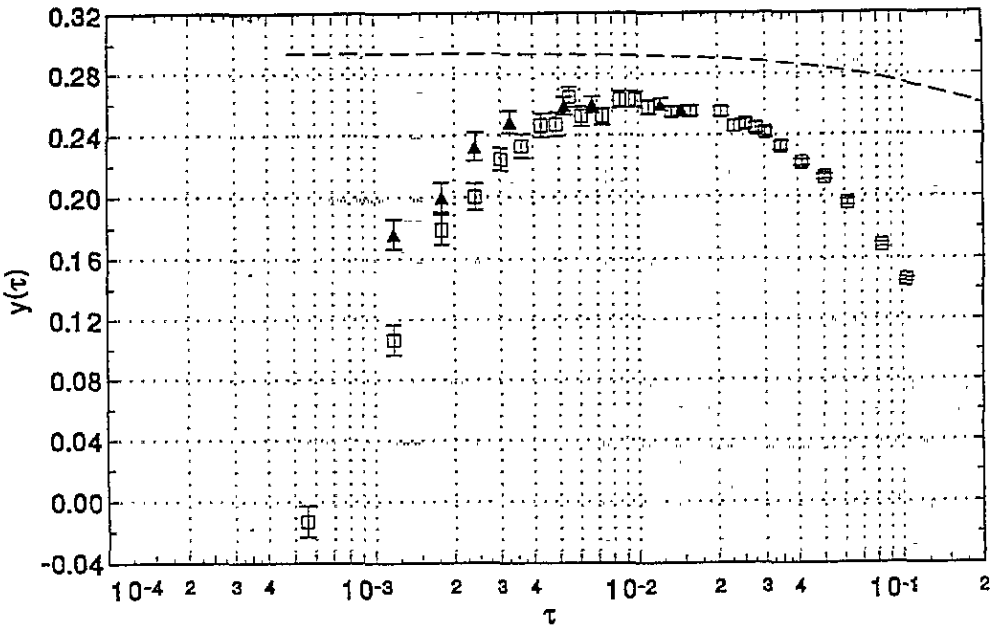

Figure 12. The difference $y(\tau)$ between $C(\tau)$ and the best logarithmic approximation for it. Pure case $y_{\text{pure}}(\tau)$ is shown by the broken line. Up triangles show $L = 1024$ impure data; empty boxes show $L = 512$ impure data.

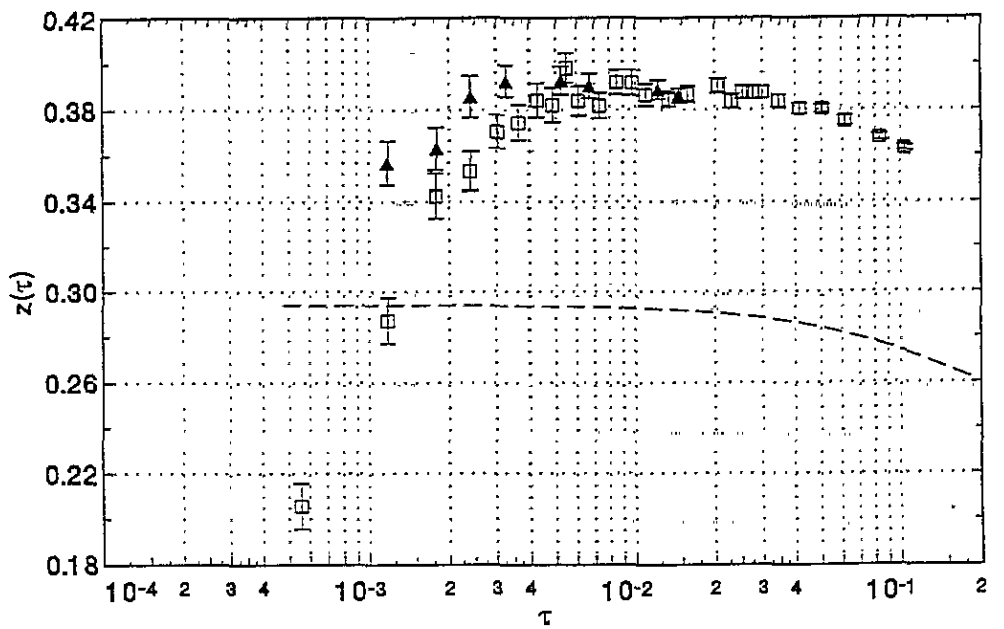

Figure 13. The difference $z(\tau)$ between $C(\tau)$ and the DD approximation for $g = 0.295$. Up triangles show $L = 1024$ data; empty boxes show $L = 512$ data. The broken line shows infinite pure system $C(\tau)$-deviations from the simple $\log(\tau)$-law. This deviations are caused by analytic corrections to scaling. The decrease of $z(\tau)$ for $\tau < 2 \times 10^{-3}$ is caused by finite-lattice effects.

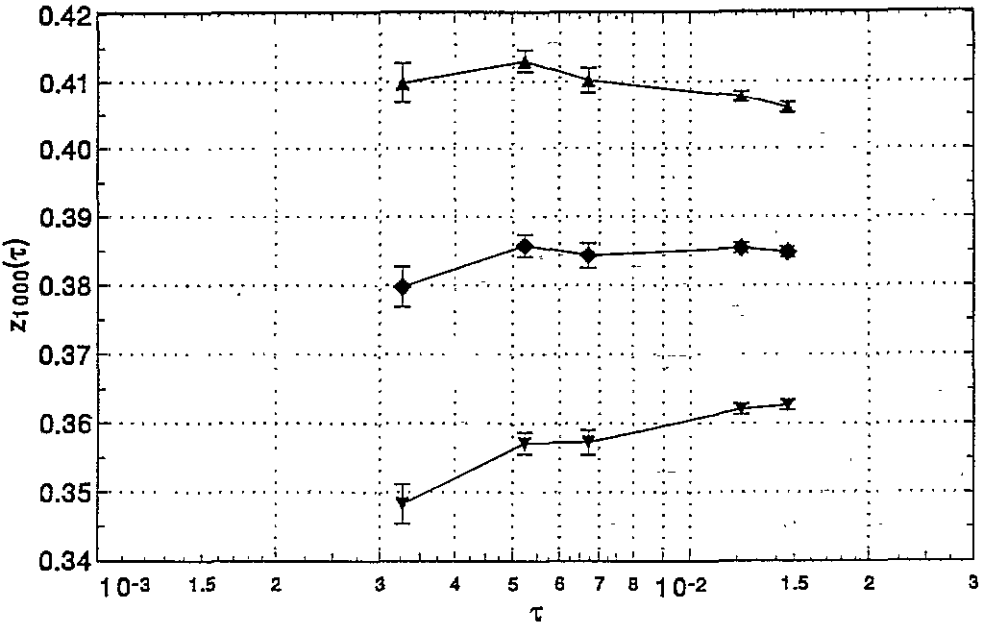

Figure 14. For 1000 samples, $L = 1024$, the critical region difference $z(\tau)$ between $C(\tau)$ and the DD approximation for $g = 0.28$ (down triangles), 0.295 (diamonds), 0.31 (up triangles).

5. Conclusions

Two alternative interpretations are compatible with our simulation results.

The first point of view is that the corrections to scaling (10) are really large, and the true asymptotic behaviour is defined by DD–SSL theory. This means that the specific heat diverges as a double logarithm of τ, while $M(\tau)$ and $\chi(\tau)$ are described by (8), (9).

The second point of view is that corrections to the scaling are negligible in the critical region (7). Then the magnetization critical exponent β and magnetic susceptibility critical exponent γ are increased by impurity. In this case the standard scaling relation $\alpha + 2\beta + \gamma = 2$ implies that the specific heat exponent α becomes negative. In our case the increase of γ is about 0.135, and the increase of β is about 0.0075. Therefore $\alpha \approx -0.15$. It turns out that the DD formula (14) with $g = 0.295$ gives practically the same results for $C(\tau)$ as the power law with $\alpha = -0.15$.

Because both contradicting interpretations agree with the simulation data, we cannot completely support the recent claim [40] that the site dilution of the 2D Ising model leads to increased value of γ. We belive that the problem can be completely resolved by simulations on much larger lattices, which will avoid the influence of analytic corrections to scaling.

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