Spin glass behavior in a random Coulomb antiferromagnet

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We study spin glass behavior in a random Ising Coulomb antiferromagnet in two and three dimensions using Monte Carlo simulations. In two dimensions, we find a transition at zero temperature with critical exponents consistent with those of the Edwards Anderson model, though with large uncertainties. In three dimensions, evidence for a finite-temperature transition, as occurs in the Edwards-Anderson model, is rather weak. This may indicate that the sizes are too small to probe the asymptotic critical behavior, or possibly that the universality class is different from that of the Edwards-Anderson model and has a lower critical dimension equal to three.

PACS numbers:

I. INTRODUCTION

Most studies of spin glasses use a model of the Edwards-Anderson [1] type in which the interactions are short-range and have random sign. However, it is argued that spin glass behavior is more general and that the necessary ingredients are simply *randomness* and *frustration*. Indeed an antiferromagnet on a random graph (which has all interactions negative) is found [2] to have spin glass behavior, in which disorder and frustration arise from large loops in the graph. In this paper we also study spin glass behavior in a disordered model with only anti-ferromagnetic interactions, but of the long-range Coulomb-type.

In addition to clarifying the general conditions under which spin glass behavior can occur, further motivation for our work comes from experiment. In certain highly frustrated random magnets, Schiffer and Daruka [3] showed that new magnetic degrees of freedom emerge, so-called "orphan" spins, which could potentially undergo a glassy transition. Subsequently, two of us and collaborators [4, 5] showed that the orphan spins have Coulomb interactions between them, due to entropic effects, and performed numerical simulations on the resulting model. A final motivation for our study is that Villain [6] showed that antiferromagnetic Coulomb interactions arise between effective Ising spins, called "chiralities", in an XY (i.e. 2-component) spin model with frustration and speculated that this could lead to a glassy transition.

The main question we address in this work is whether the spin glass transition in the random Coulomb antiferromagnet is in the same universality class as the Edwards-Anderson (EA) spin glass. Microscopically they are very different. The EA model is short-range and its interactions have random sign while the Coulomb antiferromagnet has all interactions negative and is long-range. However, Ref. [5] showed that there is a screening mechanism in the random Coulomb antiferromagnet so we might expect that the interactions driving a spin glass transition are short-range. In addition, both the EA model and the random Coulomb antiferromagnet have disorder and frustration, so one might imagine that the universal behavior at a spin glass transition could be the same. We will try to see if this is the case by numerical simulations. Our conclusion is that the data is *consistent* with this hypothesis, but other scenarios can not be ruled out because there are strong corrections to finite-size scaling for the range of sizes that we can study.

Reference [5] performed Monte Carlo simulations on a Heisenberg (i.e. three-component) version of the random Coulomb antiferromagnet because the orphan spins emerging in experimental frustrated quantum magnets [3, 4] are of the Heisenberg type. However, in order to try to answer questions about the spin glass universality class we prefer to study the Ising (i.e. one-component) version of the model. One reason is that the updating algorithm is simpler and more efficient than for the Heisenberg case. More important is that even for the EA model, the nature of the spin glass transition in, say, three dimensions has been harder to elucidate for the Heisenberg case than for the Ising case. This is partly because the transition temperature is much lower and partly because there seem to be larger corrections to finite-size scaling as well as complications due to additional (chiral) degrees of freedom, see for example Refs. [7, 8]. By contrast, the transition in the three-dimensional Ising EA spin glass is much better understood, see Refs. [9, 10]. By using Ising rather than Heisenberg spins, and by some refinements to the Monte Carlo method, we are able to study significantly larger sizes than in Ref. [5].

The plan of this paper is as follows. In Sec. II we describe the model and the numerical method used to simulate it. In Sec. III we explain the finite-size scaling method used to investigate the transition, while in Sec. IV we describe the

results and interpret them for the cases of dimension d equal to 2 and 3. Our conclusions are summarized in Sec. V.

II. THE MODEL

We study N Ising spins, $S_i = \pm 1$, randomly placed on a $d-$dimensional hypercubic lattice of size L for $d = 2$ and 3. The concentration of spins is therefore $x = N/L^d$. The Hamiltonian is given by

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J(\mathbf{r}_{ij}) S_i S_j \,, \tag{1}$$

where the interactions $J(\mathbf{r}_{ij})$ are given by the lattice Green function

$$J(\mathbf{r}_{ij}) = -\frac{a_d}{L^d} \sum_{\mathbf{k}} \frac{\cos\left(\mathbf{k}\cdot\mathbf{r}_{ij}\right)}{d - \sum_{\ell=1}^{d} \cos k_\ell} \,. \tag{2}$$

The factor a_d is introduced so that the large-distance limit has the Coulomb form

$$J(\mathbf{r}_{ij}) = \log(r_{ij}/\mathcal{L}), \qquad (d = 2), \tag{3a}$$

$$= -1/r_{ij}, \qquad (d = 3), \tag{3b}$$

where $\mathcal{L}$ is a constant which can be chosen to be larger than any r_{ij} so the interactions are all antiferromagnetic. In fact, since we impose the "charge neutrality" condition,

$$\sum_{i=1}^{N} S_i = 0, \tag{4}$$

the Hamiltonian is actually independent of $\mathcal{L}$. The numerical values of a_d are

$$a_2 = \pi, \tag{5a}$$

$$a_3 = 2\pi. \tag{5b}$$

Note that, since the *positions* of the spins are random, the interactions will be different for different samples, but always antiferromagnetic. To reduce error bars coming from sample-to-sample fluctuations we need to average over many, typically several hundred, samples.

We simulate this model using the Metropolis Monte Carlo method, modified as follows to incorporate the charge neutrality condition in Eq. (4). A site i is chosen, either sequentially or at random, and then one of the z nearest sites to this, j say, is chosen at random. If the spins on i and j are antiparallel they are both flipped with the usual Metropolis probability, and otherwise no change is made. Repeating this procedure N times corresponds to one Monte Carlo sweep. An earlier version of the code took both spins to be random, so with high probability they are far away, but this leads to an acceptance probability that decreases rapidly with increasing system size.

We incorporate parallel tempering (replica exchange) [11, 12] to speed up equilibration at low temperatures. In this approach, simulations are done at several temperatures for the same set of interactions and global moves are performed in which entire spin configurations at neighboring temperatures are exchanged, with a probability satisfying the detailed balance condition. We determine the temperatures empirically by requiring that the acceptance ratios for global moves are reasonable, typically of order 0.3. Appropriate temperatures can be estimated with sufficient accuracy from relatively short test runs.

III. QUANTITIES CALCULATED AND FINITE-SIZE SCALING

The main object of interest is the spin glass order parameter q defined as the instantaneous overlap between the spin configurations in two copies of the system with the same interactions,

$$q = \frac{1}{N} \sum_{i=1}^{N} S_i^{(1)} S_i^{(2)} \,, \tag{6}$$

where "(1)" and "(2)" refer to the copies. From measurements of q we determine the spin glass susceptibility

$$\chi_{SG} = N[\langle q^2 \rangle]_{\rm av} \tag{7}$$

and the Binder ratio

$$g = \frac{1}{2}\left(3 - \frac{[\langle q^4 \rangle]_{\rm av}}{[\langle q^2 \rangle]^2_{\rm av}}\right) , \tag{8}$$

in which angular brackets refer to a Monte Carlo average for a single sample and square brackets $[\cdots]_{\rm av}$ refer to an average over samples. It is also useful to define a wavevector-dependent spin glass susceptibility by

$$\chi_{SG}(\mathbf{k}) = \frac{1}{N}\sum_{i,j}\left[\left\langle S_i^{(1)} S_j^{(1)} S_i^{(2)} S_j^{(2)} \right\rangle\right]_{\rm av} \cos\left(\mathbf{k}\cdot\mathbf{r}_{ij}\right) , \tag{9}$$

from which one can determine a correlation length ξ_L according to

$$\xi_L = \frac{1}{2\sin(q_{\rm min})}\left(\frac{\chi_{SG}(0)}{\chi_{SG}(\mathbf{q}_{\rm min})} - 1\right)^{1/2} , \tag{10}$$

where $\mathbf{q}_{\rm min}$ is the smallest non-zero wavevector, i.e. $\mathbf{q}_{\rm min} = (2\pi/L)(1,0)$ in $d = 2$ and $\mathbf{q}_{\rm min} = (2\pi/L)(1,0,0)$ in $d = 3$.

To investigate whether or not there is a spin glass phase transition it is essential to use finite-size scaling (FSS), see for example Refs. [7, 13]. If there is a transition at $T = T_c$, in which the bulk (i.e. infinite system-size) correlation length diverges with an exponent ν, i.e.

$$\xi_\infty \propto (T - T_c)^{-\nu}, \tag{11}$$

then the Binder ratio, being dimensionless, will have the FSS form

$$g = \widetilde{g}\left(L^{1/\nu}(T - T_c)\right) , \tag{12}$$

so curves of g against T for different sizes *intersect* at T_c.

The spin glass susceptibility, however, is not dimensionless and for an infinite system size diverges at T_c with an exponent γ, i.e.

$$\chi_{SG} \propto (T - T_c)^{-\gamma}, \qquad (L \to \infty), \tag{13}$$

so its FSS form is

$$\chi_{SG} = L^{2-\eta}\,\widetilde{\chi}\left(L^{1/\nu}(T - T_c)\right) , \tag{14}$$

where η is related to the other exponents by

$$\gamma = (2 - \eta)\nu\,. \tag{15}$$

The correlation length ξ_L divided by the system size is also dimensionless and so has the FSS form

$$\frac{\xi_L}{L} = \widetilde{X}\left(L^{1/\nu}(T - T_c)\right) . \tag{16}$$

IV. RESULTS

A. Screening

The spin glass susceptibility can be expressed as

$$\begin{aligned}\chi_{SG} &= \frac{1}{N}\sum_{i,j}[C_{ij}^2]_{\rm av} \\ &= 1 + \frac{1}{N}\sum_{i\neq j}[C_{ij}^2]_{\rm av}\end{aligned} \tag{17}$$

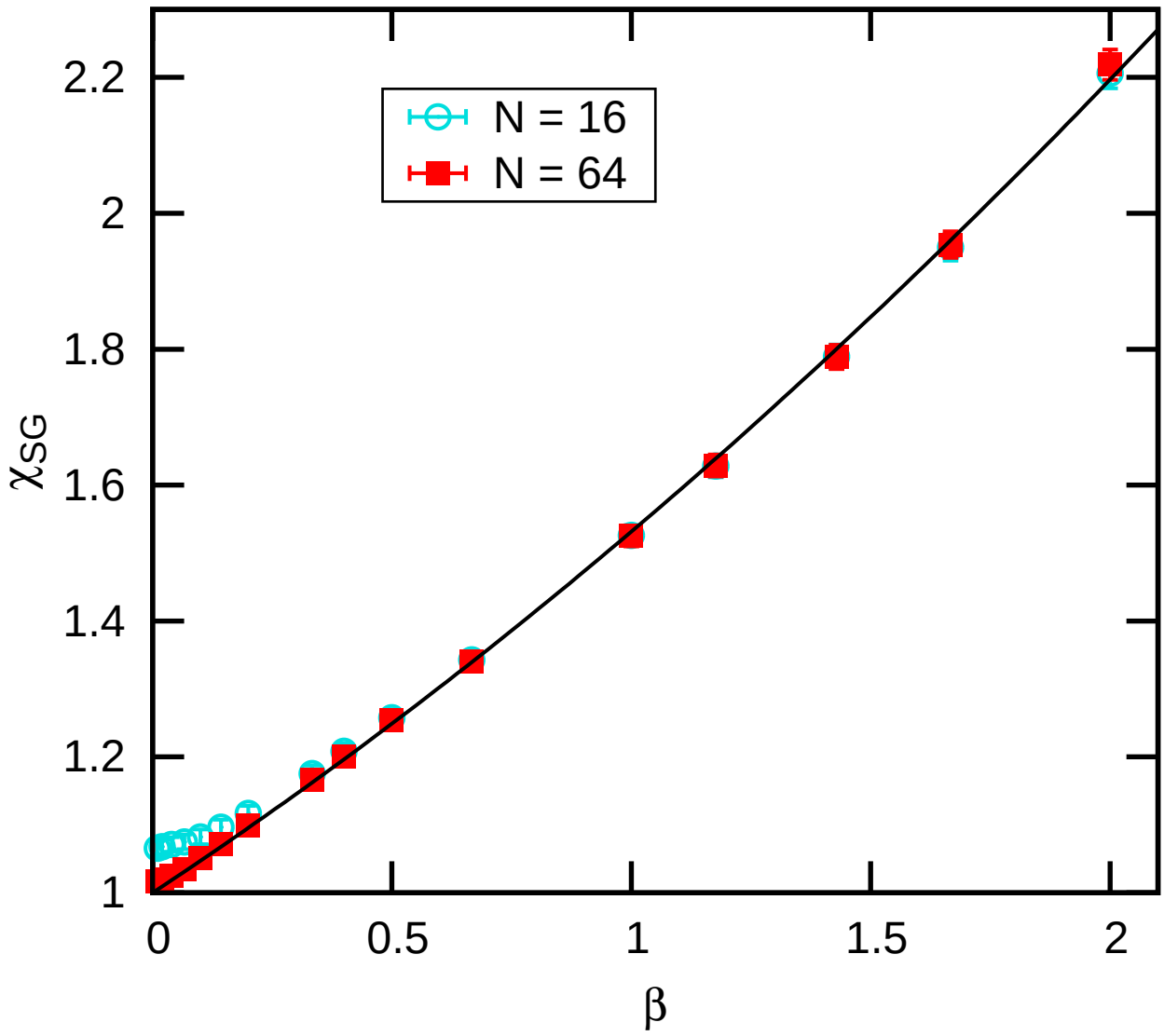

FIG. 1: Data for the spin glass susceptibility at small $\beta\,(\equiv 1/T)$ in two dimensions for a concentration $x = 1/16$ for $N = 16$ and 64. The curve is a parabolic fit to the data for $N = 64$ and has the form $1 + 0.465\beta + 0.0669\beta^2$. The behavior is clearly linear, not quadratic, at small β, which is a result of screening. The intercept at $\beta = 0$ differs measurably from unity for very small sizes only because of the charge neutrality constraint, Eq. (4).

where $C_{ij} = \langle S_i S_j \rangle$ and the terms with $i = j$ give unity, which is the result for $T = \infty$. Naively, one can obtain the second term in Eq. (17) at high temperature by expanding the Boltzmann factors in powers of $\beta\,(\equiv 1/T)$, with the result

$$C_{ij} = \beta J_{ij} + O(\beta^2) \qquad (i \neq j), \tag{18}$$

but then the sum in the second term in Eq. (17) diverges for the Coulomb potential interaction in Eq. (3). Clearly a resummation of terms is needed to get a finite result. In fact, Ref. [5] showed that the interactions are screened up to a length scale λ where

$$\lambda \propto \sqrt{T}. \tag{19}$$

Within certain approximations, the final result of Ref. [5] in $d = 2$, is

$$C_{ij} \propto \beta K_0(r_{ij}/\lambda), \tag{20}$$

where $K_0(x)$ is a modified Bessel functions which decays exponentially to zero at large x. This is to be compared with the naive result in Eq. (18) that $C_{ij} = \beta J(\mathbf{r}_{ij}) \propto \beta \log(r_{ij})$. Inserting Eq. (20) into Eq. (17) one has, at high-T and in $d = 2$,

$$\chi_{SG} = 1 + \text{const.}\, \lambda^2 \beta^2 \tag{21}$$

$$= 1 + \text{const.}'\, \beta\,. \tag{22}$$

Hence, because of screening, the leading correction to the infinite-temperature result is of order β. This is different from the naive result of high-temperature series, see Eqs. (17) and Eq. (18), which is of order β^2. However, this coefficient diverges with system size for the long-range model studied here, and a resummation of terms, which corresponds to including screening, gives a *finite* term of order β. This linear dependence at small β is clearly shown by the numerics in Fig. 1.

Because the interactions are screened, we might expect the universality class of the spin glass transition in the disordered Coulomb antiferromagnet to be the same as that of the *short-range* EA spin glass. Even if this is the case, the fact that the screening length is temperature dependent will give rise to additional, and possibly large, corrections to FSS which could complicate the analysis.

B. Equilibration

To test for equilibration we obtain data for runs of different length in which the number of sweeps doubles for each run, and for all runs we average over the last half of the sweeps. It is easy to see that this can actually be done in a single run by using *all* the data. We require that the data is independent of run time within small error bars for the last two data points. Figure 2 shows an example for $N = 576$ for $d = 2$ at the lowest temperature $T = 0.032$.

In some recent work on *very* large samples, an equilibration test is done *separately* on each sample, see e.g. [14], an approach which is useful when the sample-to-sample variation in relaxation times is huge. This variation gets larger with increasing sample size; for example the work in Ref. [14] studied samples with up to 48^3 spins. Since the sizes studied here are much smaller (only up to 10^3 spins), we expect that the variation in relaxation times will also be much smaller (though we did not test this explicitly) and so we did not perform a sample-by-sample equilibration test.

C. Two-dimensions

TABLE I: Simulation parameters for $d = 2$. The concentration is $x = 1/16$ where $N = xL^2$. For each value of size N, N_{samp} samples were run for N_{sweep} sweeps with averaging performed over the last half. Parallel tempering Monte Carlo was performed with N_T temperatures distributed between $T_{\min}$ and $T_{\max}$.

N	L	N_{sweep}	$T_{\min}$	$T_{\max}$	N_T	N_{samp}
64	32	2097152	0.025	1	15	256
144	48	2097152	0.025	0.500	15	1024
256	64	8388608	0.025	0.500	15	767
400	80	16777216	0.025	0.25	15	256
576	96	83886080	0.032	0.500	16	467
784	112	167772160	0.05	0.25	11	96

Now we discuss our results for two-dimensions. We need a concentration which is small, so we are close to the continuum limit, but not too small because then there would be some *very* strongly correlated pairs of spins which would be hard to equilibrate without a cluster-flip algorithm. We choose $x = 1/16$. The parameters of the simulations are shown Table I.

For the EA model it is well established that the spin glass transition only occurs at $T = 0$ where the correlation length diverges with an exponent $\nu \simeq 3.4$ [15–17] and the exponent η, which is related to the divergence of the spin glass susceptibility according to Eqs. (14) and (15), is $\eta = 0$.

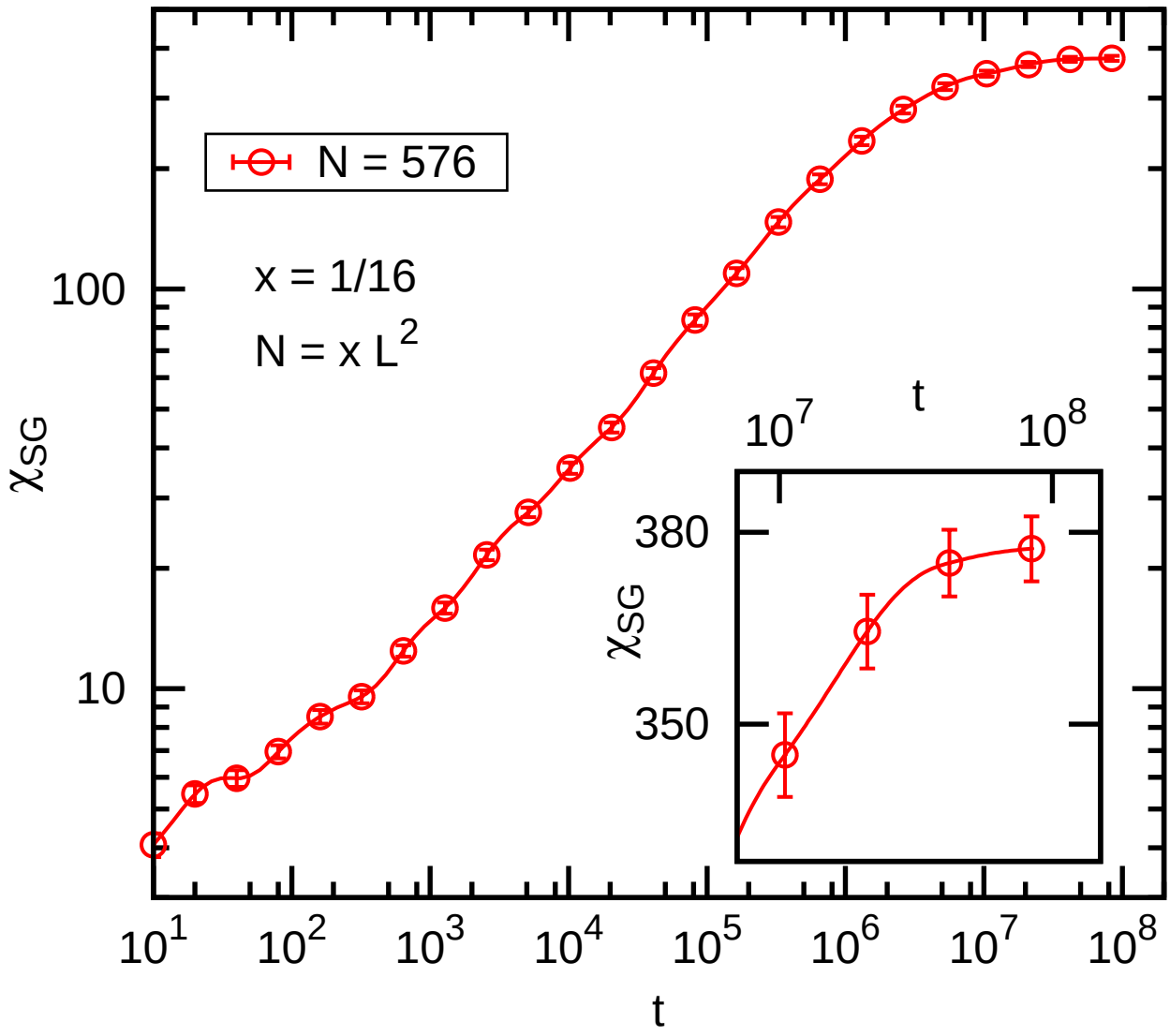

FIG. 2: Equilibration plot for $N = 576, d = 2$ with $x = 1/16$ at the lowest temperature of $T = 0.032$. The spin glass susceptibility χ_{SG} is plotted against Monte Carlo sweeps t. For each point, averaging is carried out over the last half of the sweeps. The inset shows an enlargement of the data points for the longest times.

Our data for the Binder ratio g is shown in Fig. 3. There is no sign of any intersections and hence no indication of a finite temperature transition. This is consistent with the EA model in $d = 2$. Figure 4 shows a scaling plot according to Eq. (12) assuming $T_c = 0$. If there is a zero temperature transition the data should collapse, at least for large enough sizes and low enough temperatures. We were not able to collapse the data for *all* sizes with any choice of the correlation length exponent ν but the data for the largest sizes collapses fairly well with $\nu \simeq 3.5$ (as shown) consistent with results for the EA model. However, there is a large uncertainty in this estimate; we find that any value for ν in the range 2.7 to 4.5 gives a plausible fit for large sizes.

In Fig. 5 we show scaled data for χ_{SG} according to Eq. (14) assuming $T_c = 0$ and $\eta = 0$ (the latter corresponding to a non-degenerate ground state which seems reasonable). As with the data for g in Fig. 4, we can not scale all the data for any value of ν. However, the data for larger sizes scales fairly well with a value of 2.7 (shown) not very different from the value for the EA model of 3.4. However, there are big uncertainties in our estimate; any value between 2.0 and 4.0 gives a plausible collapse for large sizes.

Our attempts to scale the data for g and χ_{SG} indicate the presence of substantial corrections to FSS for the range of sizes that we can study. This problem is even more severe for the data for ξ_L/L. Being dimensionless, the data

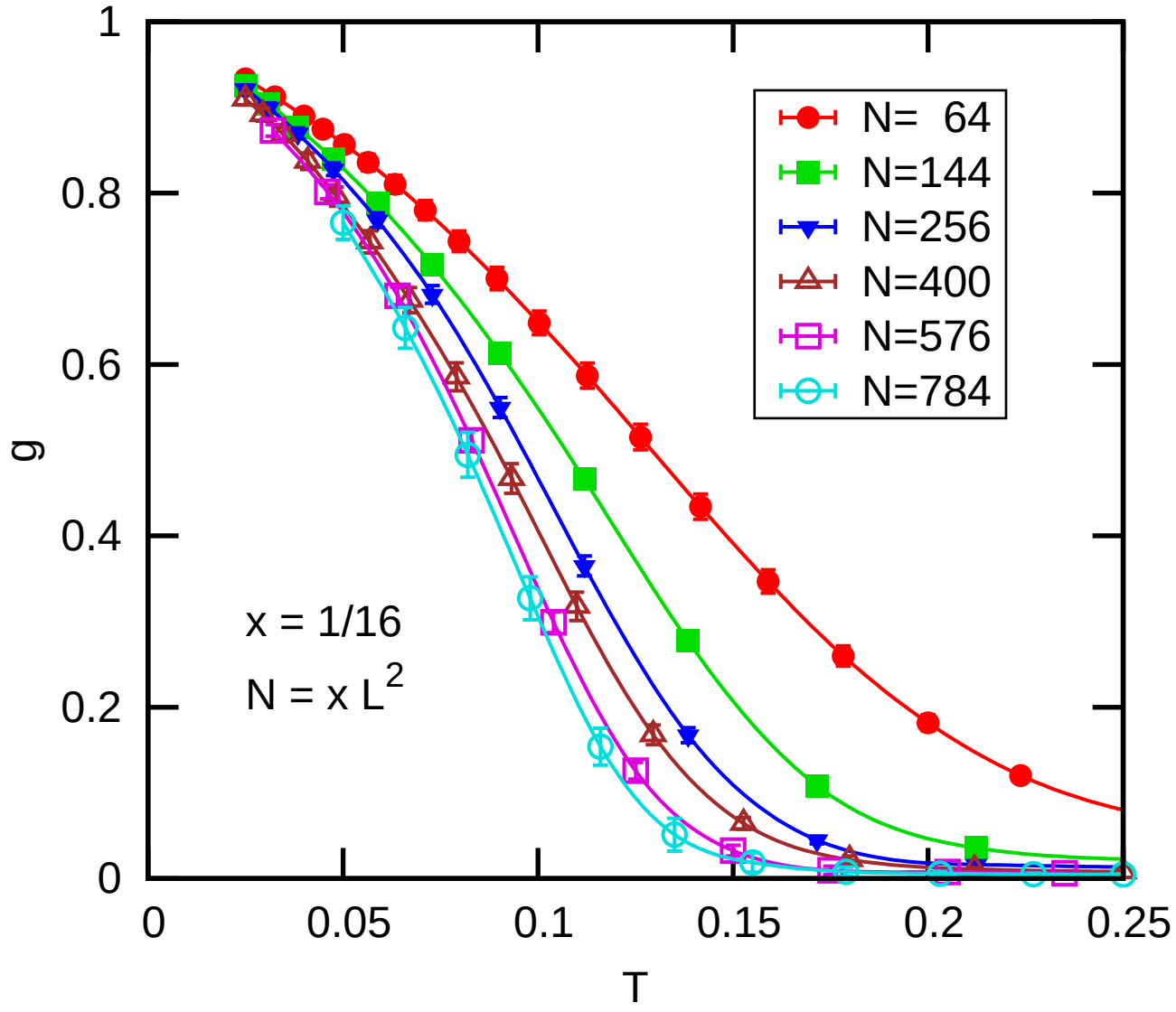

FIG. 3: Data for the Binder ratio in $d = 2$.

for this quantity should intersect if there is a transition, see Eq. (16). As shown in Fig. 6 there *is* an intersection involving the smallest size studied, $N = 64$, but not for larger sizes. Rather the data for larger sizes seems to merge at low-T. If we try to scale the data for ξ_L/L we need a large value of ν to collapse the data for large sizes. Figure 7 shows the result with $\nu = 5.0$. These results indicate that the data for ξ_L/L is not at large enough sizes to give a clear prediction for the nature of the transition.

To help clarify the extent of corrections to finite-size scaling, we have plotted the two dimensionless quantities, g and ξ_L/L *against each other*, rather than separately against T. In the absence of scaling corrections the data should collapse on to a single curve. Our results are presented in Fig. 8 and they show, as suspected above, that there are strong corrections for sizes $N = 64$ and 144 but rather weak corrections for the larger sizes.

D. Three-dimensions

Next we discuss our results for three-dimensions for which we use a fixed concentration $x = 1/64$. As for $d = 2$ we choose a value which is small but not too small. For both dimensions the value of x is such that the mean spacing in each direction is 4 lattice spacings. The parameters of the simulations are shown Table II. For the EA model in

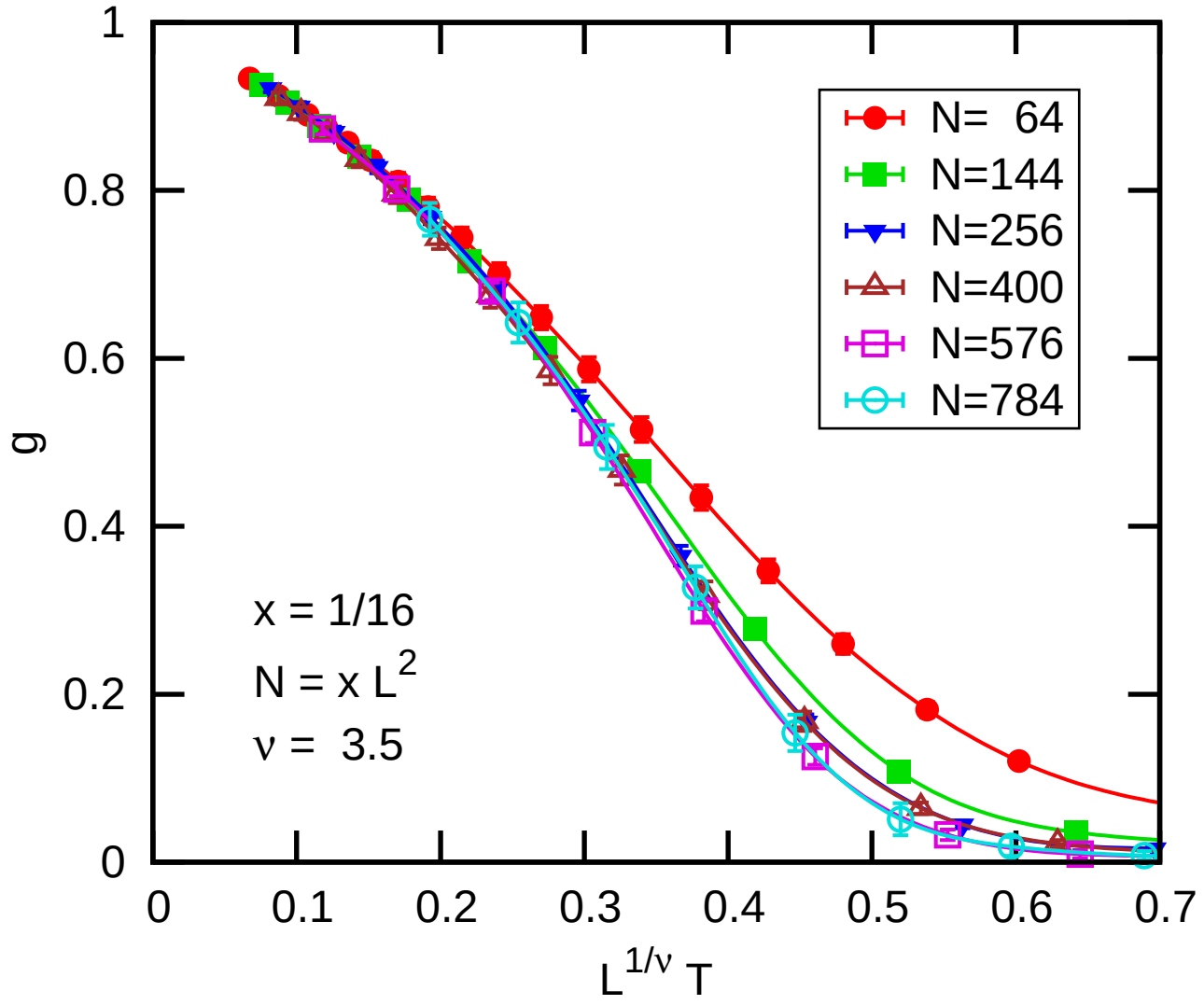

FIG. 4: Scaling plot for Binder ratio in $d = 2$ according to Eq. (12) with $T_c = 0$. We are not able to get *all* the data to collapse for any value of the correlation length exponent ν. However the data for the largest sizes collapses with $\nu \simeq 3.5$ (shown), consistent with the value in the EA model. However, there are big uncertainties in our estimate (see text).

$d = 3$ it is firmly established that there is a spin glass transition at non-zero temperature [9, 10].

Data for the dimensionless quantities g and ξ_L/L are shown in Figs. 9 and 10 respectively. The results for g seem to merge at low-T but do not obviously cross. It should be mentioned that even for the EA model the splaying out of the data for g below T_c is only a small effect, see for example Ref. [18], but is, nonetheless, observable with good data on large sizes.

For small sizes the data for ξ_L/L shows a large splaying out, but the data for large sizes seems only to merge. Splaying out for the smallest size was also observed in $d = 2$, see Fig. 6, and was interpreted as a FSS correction since it disappears for larger sizes. The same is presumably true here; we should give most weight to the data for larger sizes. But the larger size data in Fig. 10 looks very marginal, possibly suggesting that $d = 3$ is the lower critical dimension, d_l. This is different from the EA model where d_l is approximately, or possibly exactly [19], equal to 2.5.

Figure 11 shows a plot of g against ξ_L/L, analogous to Fig. 8 for $d = 2$. The data shows that there are very large corrections to scaling for $N = 64$ but these are much smaller for the larger sizes, especially for $N \geq 512$. This conclusion is consistent with the data in Figs. 9 and 10 which plot each of these quantities separately against temperature.

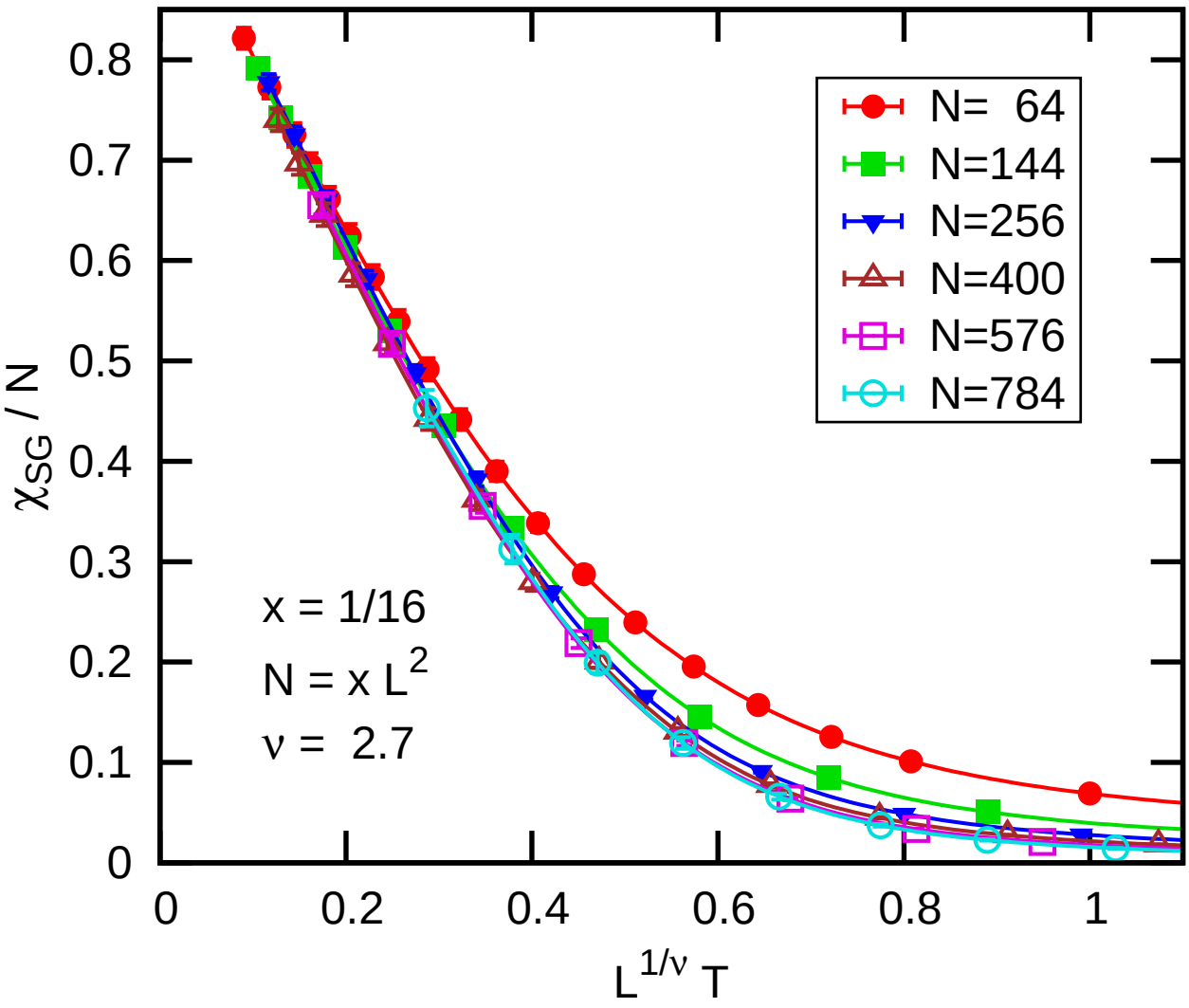

FIG. 5: The spin glass susceptibility in $d = 2$ scaled according to Eq. (14) with $T_c = 0$ and $\eta = 0$. No value of ν succeeds in scaling all the data though the largest sizes scale reasonably well with $\nu \simeq 2.7$ (shown), not very different from the value for the EA model of 3.4. However, there are big uncertainties in our estimate (see text).

V. CONCLUSIONS

We have studied spin glass behavior in the random Coulomb Ising antiferromagnet in two and three dimensions by Monte Carlo simulations, with results analyzed by FSS. Since the interactions are screened, and so are effectively short-ranged, a natural hypothesis is that the critical behavior is the same as that of the short-range Ising EA model. For the latter, a transition occurs at $T = 0$ in $d = 2$ but at a non-zero temperature in $d = 3$. Our results indicate a zero temperature transition in $d = 2$, with a correlation length exponent compatible with that found for the EA model, though with big error bars. However, in $d = 3$, we do not find unambiguous evidence for a non-zero temperature transition temperature. Rather the data for larger sizes seems to be "marginal". This could indicate that the system sizes are simply not large enough to see the asymptotic critical behavior, or it could be that our model is *not* in the same universality class as that of the short-range Ising EA model, but rather has a different lower critical dimension, $d_l = 3$ rather than $d_l = 2.5$ for the EA model. If this is the case, the nature of the physics causing the difference in universal behavior is unclear to us.

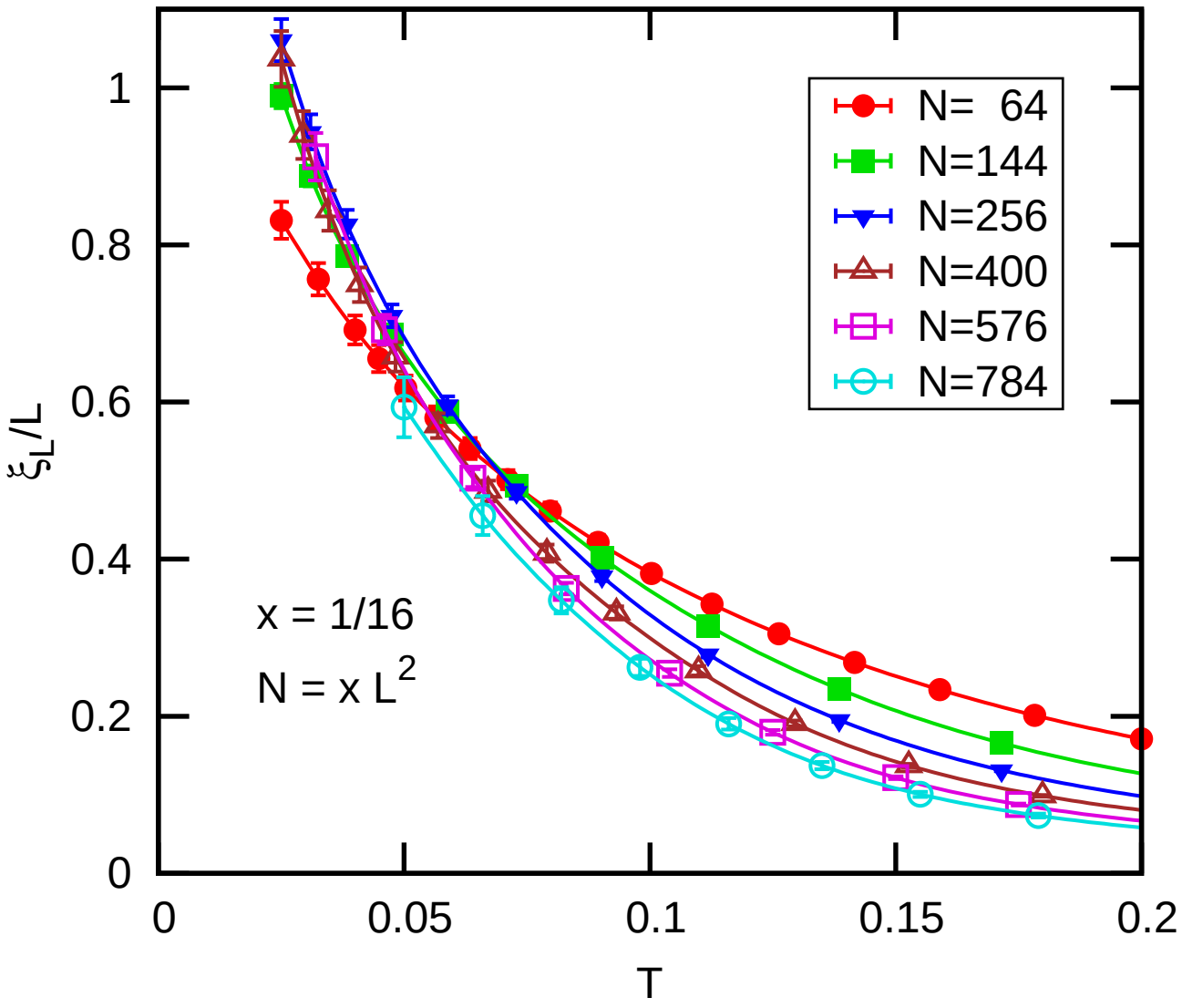

FIG. 6: Correlation length divided by system size in $d = 2$.

There are clearly large corrections to FSS for this problem. This is particularly evident in Figs. 8 and 11 which plot one dimensionless quantity, the Binder ratio g, against another dimensionless quantity, the correlation length ξ_L divided by system size. The lack of data collapse for smaller sizes shows *directly* the presence of corrections to FSS, without needing to adjust any parameters such as critical exponents. As well as corrections to scaling that occur for the short-range EA model, here we have an additional contribution because the screening length is *temperature-dependent*. In fact, according to Ref. [5] the screening length is singular for $T \to 0$, see Eq. (19). If this result holds down to $T = 0$ it could possibly *change* the critical behavior in $d = 2$, where the transition is also at zero temperature, rather than simply giving a *correction* to scaling. In $d = 3$, the transition is at finite-T for the EA model, so we expect only a correction to scaling from the T-dependence of λ.

We close on a historical note. The question of whether or not there is a finite temperature transition in the $d = 3$ Ising EA spin glass was controversial for many years. It was only later, when better FSS methods were developed and computers became more powerful, that the question was definitely answered in the affirmative. Perhaps, therefore, it is not surprising that this early effort on a Coulomb spin glass does not leave to a definite conclusion, given the extra difficulties of long-range interactions and larger corrections to scaling.

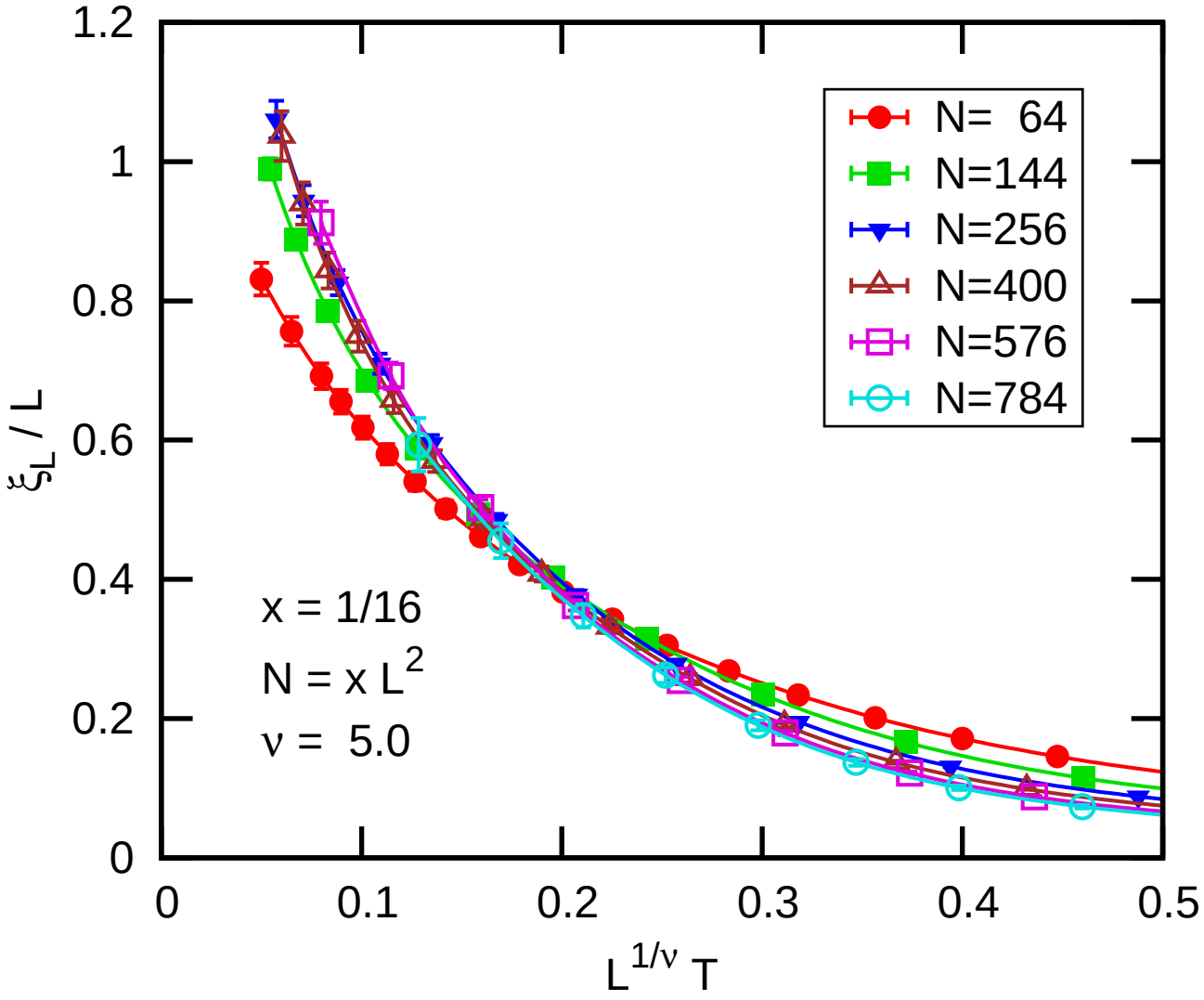

FIG. 7: Scaling plot of the correlation length divided by system size in $d = 2$ assuming $\nu = 5.0$.

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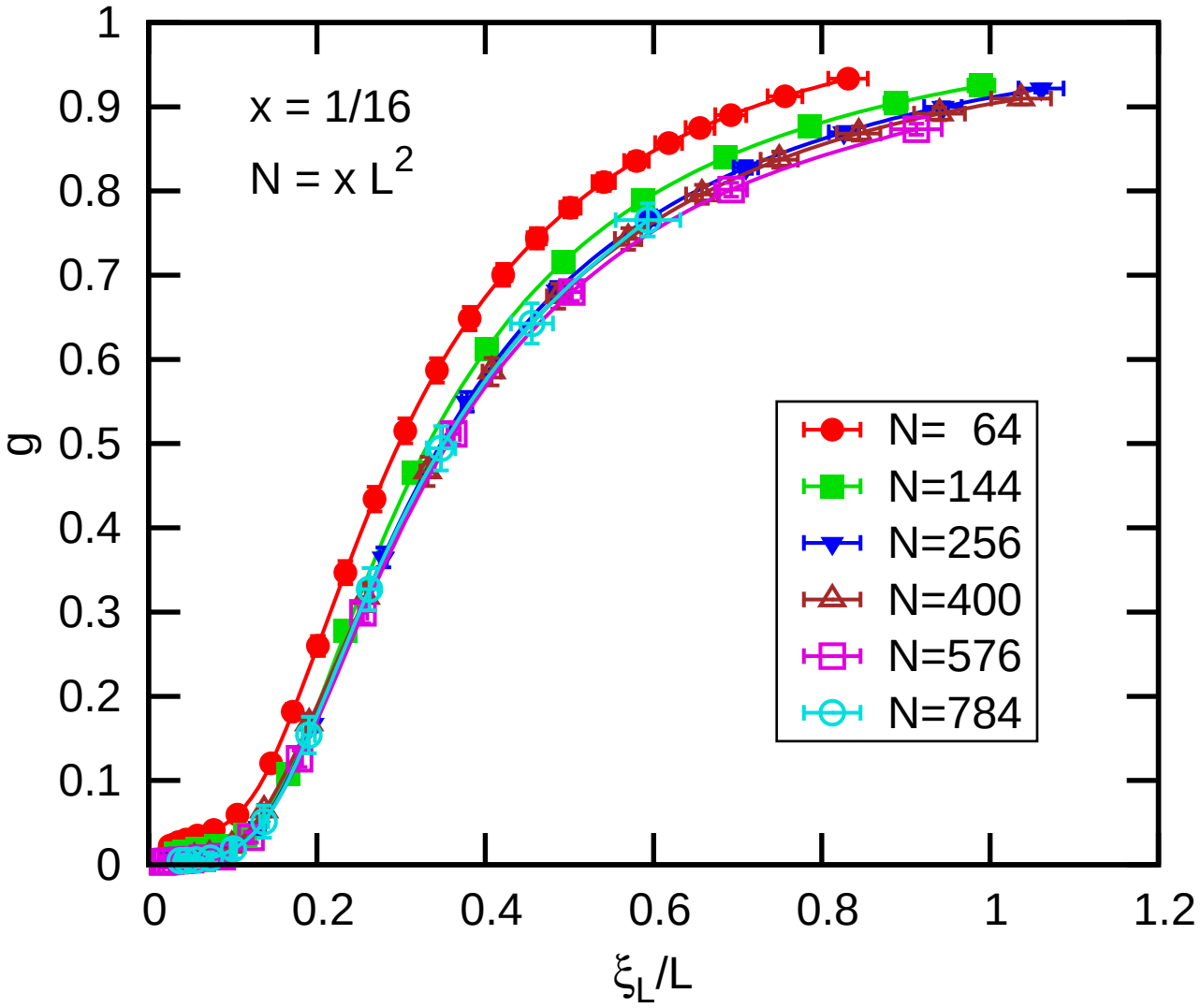

FIG. 8: A plot of the Binder ratio against the correlation length divided by (linear) system size L for different values of N. Since both these quantities are dimensionless, the data should collapse in the absence of corrections to finite-size scaling. The results show that corrections are large for $N = 64$, moderate for $N = 144$ and quite small for the larger sizes.

TABLE II: Simulation parameters for $d = 3$. The concentration is $x = 1/64$ where $N = xL^3$. For each value of size N, $N_{\rm samp}$ samples were run for $N_{\rm sweep}$ sweeps with averaging performed over the last half. Parallel tempering Monte Carlo was performed with N_T temperatures distributed between $T_{\rm min}$ and $T_{\rm max}$.

N	L	$N_{\rm sweep}$	$T_{\rm min}$	$T_{\rm max}$	N_T	$N_{\rm samp}$
64	16	20480	0.0100	0.2000	9	1000
216	24	1310720	0.0100	0.2000	12	400
512	32	41943040	0.0200	0.2150	15	360
1000	40	83886080	0.0215	0.1305	15	568

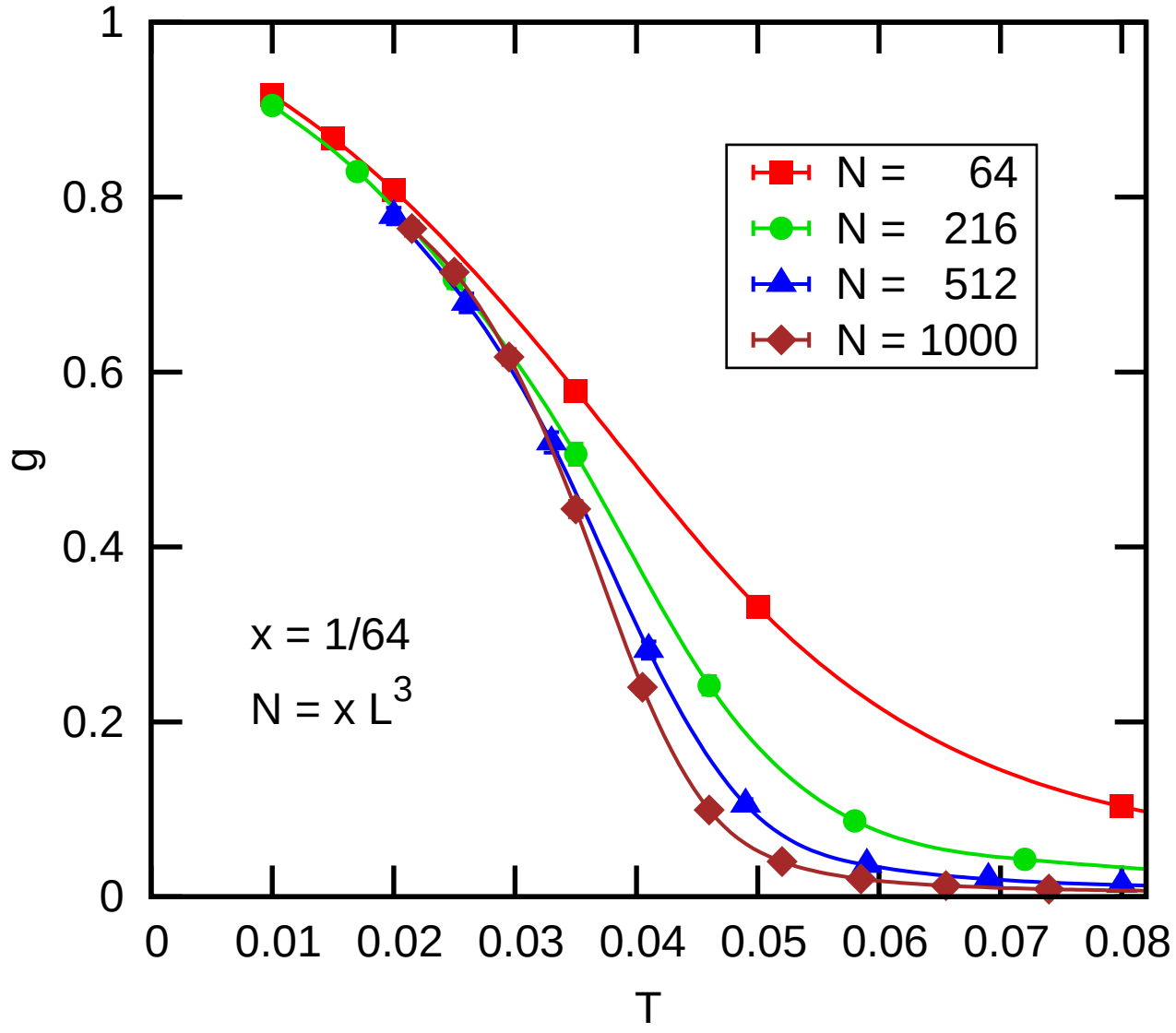

FIG. 9: Binder ratio for $d = 3$.

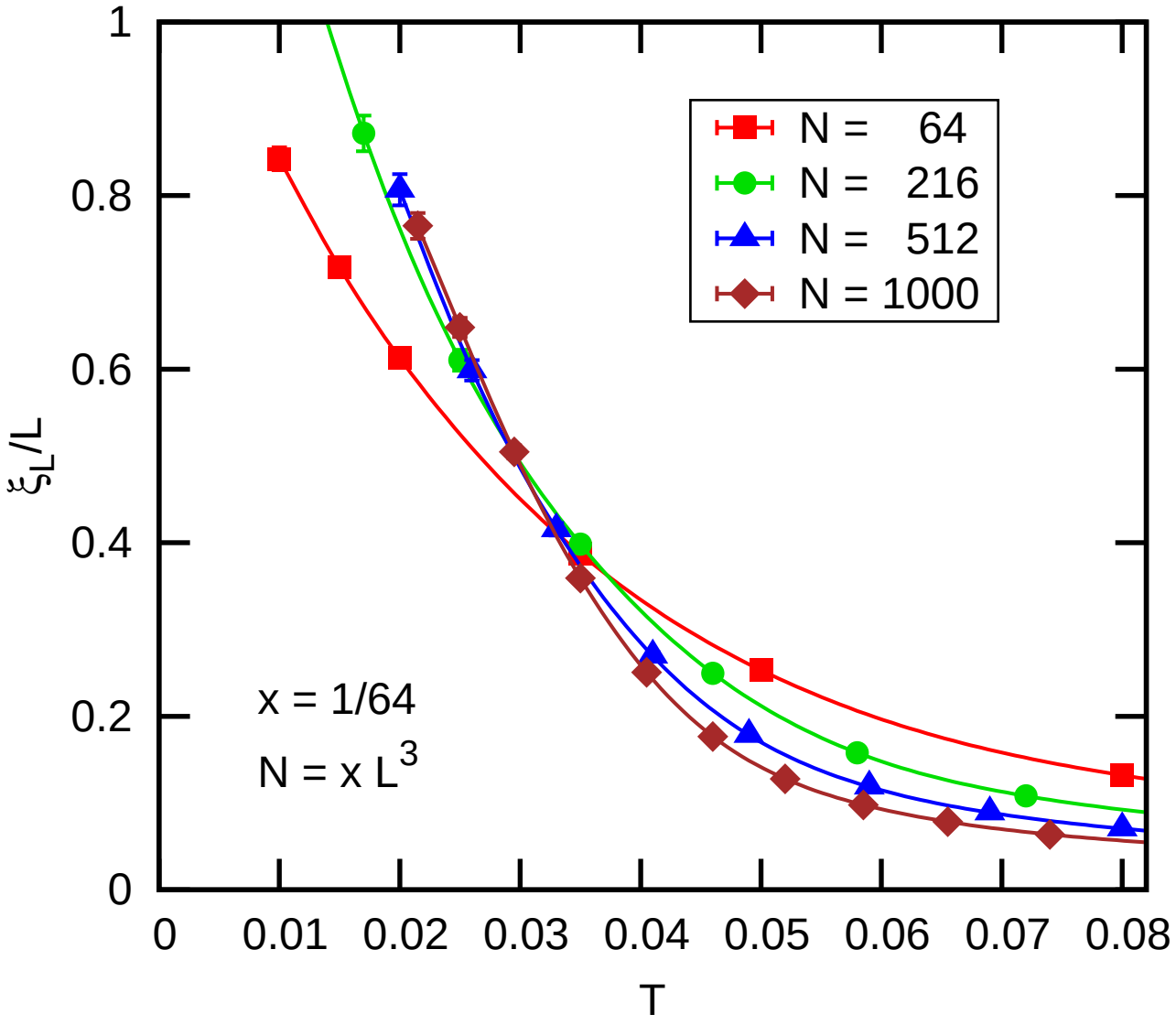

FIG. 10: Correlation length divided by system size for $d = 3$.

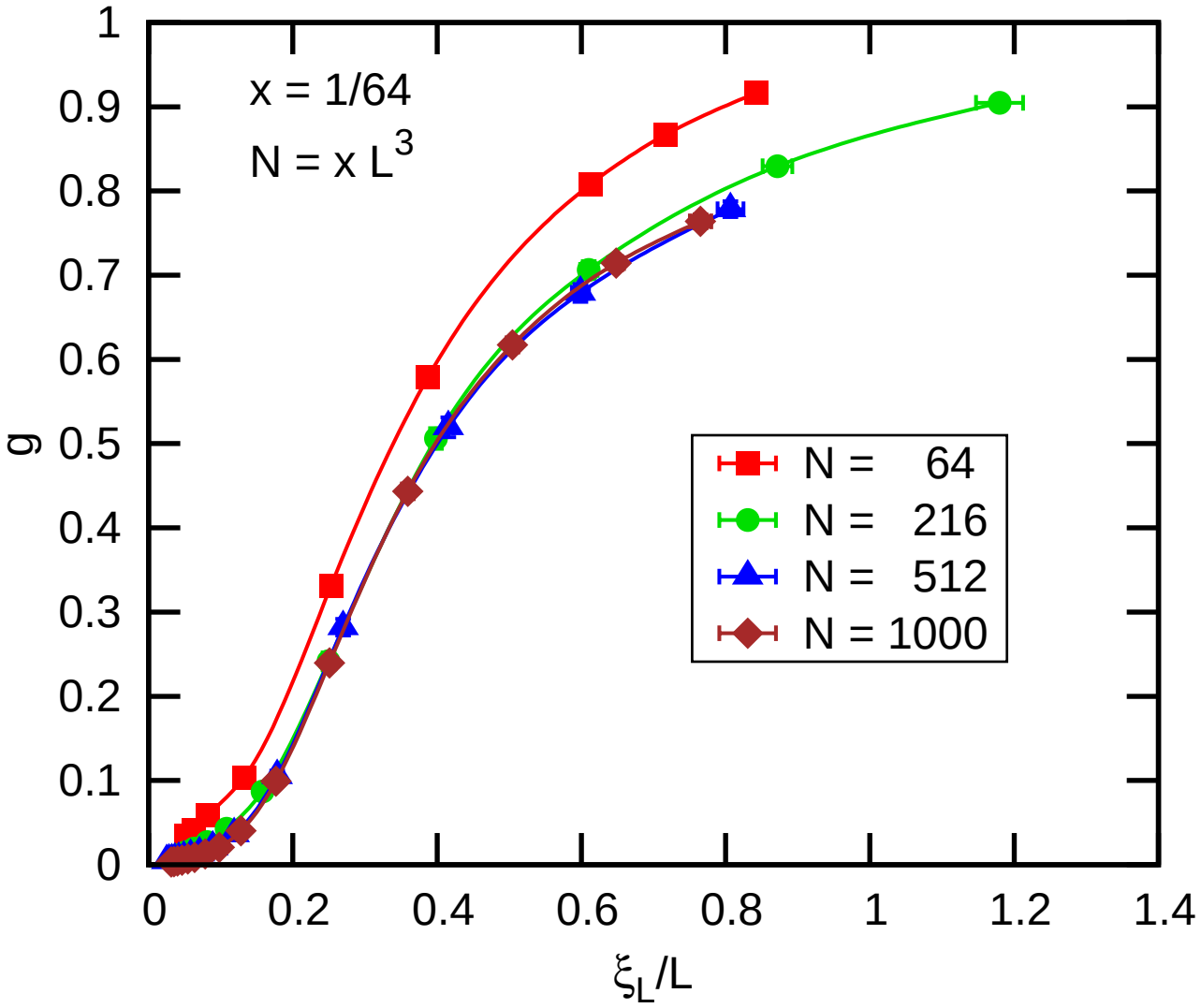

FIG. 11: A plot of the Binder ratio against the correlation length divided by (linear) system size L for different values of N. Since both these quantities are dimensionless, the data should collapse in the absence of corrections to finite-size scaling. The results show that corrections are very large for $N = 64$, moderate for $N = 216$ and apparently quite small for the larger sizes.

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