BRIEF REPORTS

Brief Reports are accounts of completed research which do not warrant regular articles or the priority handling given to Rapid Communications; however, the same standards of scientific quality apply. (Addenda are included in Brief Reports.) A Brief Report may be no longer than four printed pages and must be accompanied by an abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.

Self-averaging of random and thermally disordered diluted Ising systems

Manuel I. Marqués and Julio A. Gonzalo*
Departamento de Física de Materiales, C-IV, Universidad Autónoma de Madrid, 28049 Madrid, Spain
(Received 20 January 1999)

Self-averaging of singular thermodynamic quantities at criticality for randomly and thermally diluted three-dimensional Ising systems has been studied by the Monte Carlo approach. Substantially improved self-averaging is obtained for critically clustered (critically thermally diluted) vacancy distributions in comparison with the observed self-averaging for purely random diluted distributions. Critically thermal dilution, leading to maximum relative self-averaging, corresponds to the case when the characteristic vacancy ordering temperature (θ) is made equal to the magnetic critical temperature for the pure three-dimensional (3D) Ising systems (T_c^{3D}). For the case of a high ordering temperature ($\theta \gg T_c^{3D}$), the self-averaging obtained is comparable to that in a randomly diluted system. [S1063-651X(99)11008-0]

PACS number(s): 05.50.+q, 75.10.Nr, 75.40.Mg, 75.50.Lk

Systems with quenched randomness have been studied intensively for several decades [1]. One of the first results was the establishment of the Harris criterion [2], which predicts that weak dilution does not change the character of the critical behavior near second order phase transitions for systems of dimension d with specific heat exponent lower than zero (so called P systems), $\alpha_{\text{pure}} < 0 \Rightarrow \nu_{\text{pure}} > 2/d$, in the nonrandom case. This criterion has been supported by several renormalization group (RG) analyses [3–5], and by scaling analysis [6]. It was shown to hold also with strong dilution by Chayes *et al.* [7]. For $\alpha_{\text{pure}} > 0$ (called R systems); for example, the Ising 3D case, the system fixed point flows from a pure (undiluted) fixed point towards a new stable fixed point at which $\alpha_{\text{random}} < 0$ [3–8].

For a random hypercubic sample of linear dimension L and number of sites $N = L^d$, any observable singular property X presents different values for the different realizations of randomness corresponding to the same dilution. This means that X behaves as a stochastic variable with average $[X]$, variance $(\Delta X)^2$, and a normalized square width $R_X = (\Delta X)^2/[X]^2$. A system is said to exhibit self-averaging (SA) if $R_X(L) \rightarrow 0$ as $L \rightarrow \infty$. If the system is away from criticality, $L \gg \xi$, ξ being the correlation length, the central limit theorem indicates that strong SA must be expected. However, the behavior of a ferromagnet at criticality, where $\xi \gg L$, is not so obvious. This point has been studied recently. Wiseman and Domany (WD) investigated the self-averaging of diluted ferromagnets at criticality by means of finite-size scaling calculations [9], concluding weak SA for both the P and R cases. In contrast Aharony and Harris (AH), using a renormalization group analysis in $d = 4 - \epsilon$ dimensions, proved the expectation of a rigorous absence of self-averaging in critically random ferromagnets [10]. More recently, WD used Monte Carlo simulations to check the lack of self-averaging in critically disordered magnetic systems [11]. The absence of self-averaging was confirmed. The source of the discrepancy with their previous scaling analysis was attributed to the particular size dependence of the distribution of pseudocritical temperatures used in their work.

Quenched randomness has been investigated basically under two different constraints, a grand-canonical constraint [average density of occupied spin sites (p) fixed] and a canonical constraint [total number of occupied sites (c) constant]. The applicability of the result obtained by Chayes *et al.* also to canonical ensembles, implying universality between both kinds of constraints, has been recently investigated [12,13]. Monte Carlo simulations [11,13] indicate universality for R_X in the grand-canonical ensembles with different concentrations (p). Universality between results obtained in the canonical and the grand-canonical constraints at very large values of L is implied by the work of Aharony *et al.* [13].

In all cases previously investigated frozen disorder was always produced in a random way; that is, vacancies were distributed throughout the lattice randomly. Real systems, however, can be realized in other kinds of vacancy distributions. In particular, dilution in a ferromagnetic lattice can be produced by an equilibrium thermal order-disorder distribution of vacancies, governed by a characteristic ordering temperature (θ). If this ordering temperature θ is high enough, the equilibrium thermal disorder will be similar to the random disorder of previous investigations. However, if θ happens to coincide with the characteristic magnetic critical temperature ($T_c^{3D} = 4.511617$) of the undiluted system, new possibilities are open. In the present work we study the ef-

*Author to whom correspondence should be addressed. FAX: 34-91-3978579. Electronic address: julio.gonzalo@uam.es

fects on the magnetization self-averaging in diluted ferromagnets obtained by thermal vacancy distributions in three-dimensional Ising systems using the Monte Carlo approach. We will study the self-averaging or lack of it in these systems and will compare the results with those obtained with random vacancy distributions for the same concentration.

In order to actually produce these so called thermally diluted systems we take the following steps: First we thermalize the pure system at a given temperature (θ), finding a number N_+ of (+) sites and a number N_- of (−) sites in thermal equilibrium. Then we consider the minority kind, either (+) or (−) and we label them as vacancies, thereafter freezing in the disordered system. Only sites of the majority kind will be occupied by spins. Once the spin system has been prepared in this way, we can study any singular magnetic physical property at a given temperature (T).

The spin system (i) so constructed will have a magnetic site concentration $c_i = |N_s|/N$, where N_s is the number of majority spins from the pure system and $N = N_+ + N_-$ is the total number of sites. For a large enough value of L and $\theta \geqslant T_c^{3D}$, c_i will approach 0.5 in most cases.

We perform Monte Carlo calculations of the magnetization per spin at criticality for systems thermally and randomly diluted, using in both cases the Wolff [14] single cluster algorithm [15] with periodic boundary conditions, on lattices of different sizes L. Determinations of the magnetic critical temperature for different dilutions $[T_c(p)]$ were in good agreement with those previously given with high accuracy by Heuer [16] and by Wiseman *et al.* [11].

We consider thermally diluted samples at two different values of θ ($\theta = 4.5115 = T_c^{3D}$ and $\theta = 1000 \gg T_c^{3D}$) for the same value of $L = 40$. We can compare this thermal distributions of vacancies with the equivalent random distribution with probability $p = 0.5$. We will consider the magnetization per spin for each sample at criticality; that is, the magnetization $M_i[T_c(p)]$ for each realization ''i'' within the full set of samples. In order to show at a glance the resulting dispersion in c and in M, we use a scattered plot c vs M, where each point on the plane represents an actual realization of a given density of spins c_i and a given magnetization per spin M_i. This plot contains more information than the usual histograms.

First we consider what we may call the *hypercritical* case where $\theta = 1000$. Results are shown in Fig. 1 for $L = 40$. As expected, both diluted sets realized by thermal and random dilution look almost the same, showing the equivalent effects of a high ordering temperature and random dilution. Histograms for the magnetization are shown, at the ''grand-canonical'' case with $p = 0.5$ and $c > 0.5$ (in our realizations, there are never more vacancies than spins). Similar normalized square widths are found, $R_M^{\mathrm{random}} \approx R_M^{\mathrm{thermal}} \approx 0.06$ in both cases. They are smaller than the ones on Ref. [13] due to the fact that for us $c > 0.5$ always.

Next we consider the *critical* case, $\theta = T_c^{3D}$. Results are shown in Fig. 2 again for $L = 40$. The situation changes completely. Now the critically thermally ordered set behaves differently, with an increase in the dispersion in c. The magnetization has been calculated at the *critical* temperature for a dilution equal to $p = 0.5$, $T_c(p = 0.5)$ in order to compare the normalized square width in both cases. In this case we find

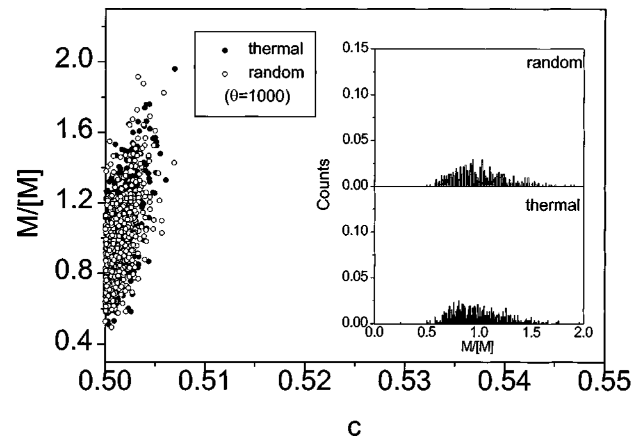

FIG. 1. Scattered plot of the concentration of spins (c) versus the normalized magnetization per spin $M/[M]$. ($[M]$ is the media of the magnetization in all the realizations: $[M]^{\mathrm{random}} \approx [M]^{\mathrm{thermal}} \approx 0.15$.) Results are shown for the random case with $p = 0.5$ and $c \geqslant 0.5$ (open circles) and the hypercritical thermal case with $\theta = 1000 \gg T_c^{3D}$ (black circles). Dispersion of the magnetization and dispersion of the concentration are similar in both cases. The inset shows the histograms for the values of the normalized magnetization in both dilutions. The upper case corresponds to *random* dilution and the lower to *thermal* dilution. Note the equivalence of the shapes resulting in similar values for the normalized square widths.

extremely low values of the normalized square width for the thermally diluted set of samples in the ''grand-canonical'' case, $R_M^{\mathrm{thermal}} \approx 10^{-3}$, which is around 60 times smaller than the width found for the random case. (See the width differences in the histograms on Fig. 2).

To study the self-averaging evolution we must consider the behavior of the normalized square with R_M with the length L of the system. Consequently we have diluted the

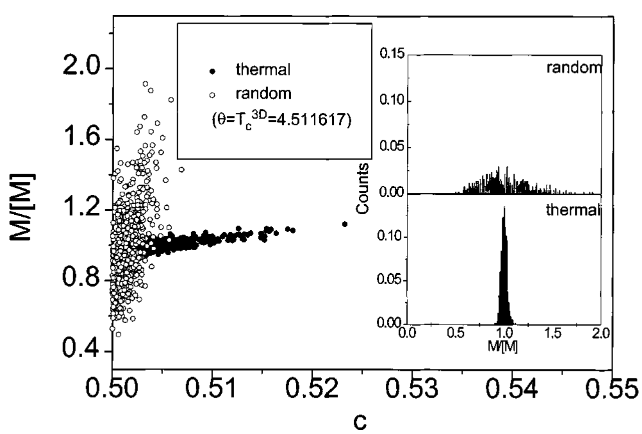

FIG. 2. Scattered plot of the concentration of spins (c) versus the normalized magnetization per spin $M/[M]$: $[M]^{\mathrm{random}} \approx 0.15$; $[M]^{\mathrm{thermal}} \approx 0.6$. Results are shown for the random case with $p = 0.5$ and $c \geqslant 0.5$ (open circles) and the critical thermal case with $\theta = T_c^{3D} = 4.511617$ (black circles). Dispersion of the magnetization data is increased in the random dilution case and dispersion of the concentration is increased in the thermal disposition. The inset shows the histograms of the values for the normalized magnetization in both cases. The upper case corresponds to random dilution and the lower one to thermal dilution. Note the difference of the shapes resulting in different values of the normalized square widths.

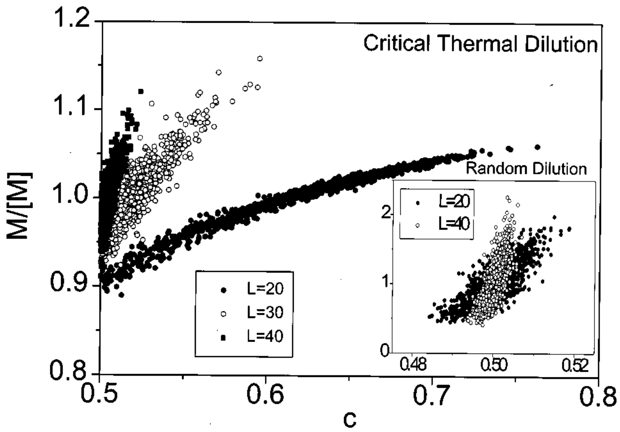

FIG. 3. Scattered plot of the concentration of spins (c) versus the normalized magnetization per spin $M/[M]$ for critical random dilution at different lengths (L), $L=20$ (black circles), $L=30$ (open circles), and $L=40$ (black squares). We find $[M]^{\mathrm{thermal}}\approx 0.9$ for $L=20$, $[M]^{\mathrm{thermal}}\approx 0.7$ for $L=30$, and $[M]^{\mathrm{thermal}}\approx 0.6$ for $L=40$. Note the decrease in the dispersion of c as L increases. This behavior means that, as L increases, the system tends to a constant value of $c=0.5$ corresponding to the canonical constraint. The inset shows the same scattered plot but now for the random case with $p=0.5$ and $L=20$ (black circles) and $L=40$ (open circles).

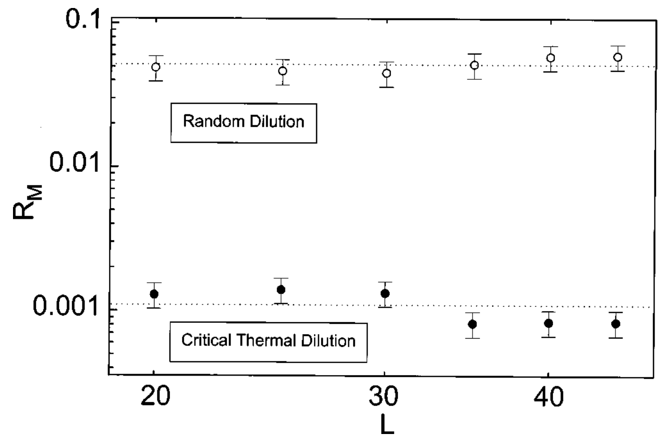

FIG. 4. Log-log plot of the normalized squared width of the magnetization R_M versus the length L of our system for the ''grand canonical'' case. Results are shown for the random dilution with $p=0.5$ and $c\geqslant 0.5$ (open circles) and for the critically thermally dilution (black circles).

systems thermally at criticality ($\theta=T_c^{3\mathrm{D}}$) for different values of L. Of course, in all these realizations for critical thermal cases, the corresponding value of p depends on the value of L, but tends always to 0.5 as L increases as it should. We have then calculated the magnetization for $T=T_c(p=0.5)$ in order to compare the evolution of the normalized square widths of the thermally diluted cases under the ''grand-canonical'' constraint with the respective widths corresponding to random dilution with $p=0.5$.

The evolution with L of the full scattering plot (M vs c) for the critical thermal case is presented on Fig. 3. Note how the evolution with increasing L of the ''cloud'' of points reduces the dispersion in the values of c, and the ''cloud'' tends to that for the canonical case, as should be, according to [13]. This behavior is also appreciable for random dilution, even when the decrease in the dispersion on c is not so easily seen, due to the restriction to $p=0.5$ only (see inset in Fig. 3). A more accurate statistical study will be needed to investigate quantitatively the behavior of R_M with the dimension L of our system, and, in agreement with Ref. [13] higher values of L will be needed to find total universality of behavior between canonical and grand-canonical constraints.

The main result of this study is the substantial improvement in the self-averaging using a thermal distribution of vacancies for all L values considered under the ''grand-canonical'' constraint with $p=0.5$ and $c\geqslant 0.5$. The normalized squared width R_M of the magnetization is always around one order of magnitude bigger for the random case than for the critically thermally diluted disposition of vacancies (see Fig. 4).

Intuitively, an equilibrium thermal distribution of vacancies at criticality implies a clustered distribution of both spins and vacancies for a given distribution level (p,c). This implies an increase in the relative number of bonds between neighboring spins, and therefore an increase of the ordering and a subsequent decrease of the normalized square width for the magnetization.

We can summarize our results as follows: using the Monte Carlo approach we have investigated diluted ferromagnets using a new method to specify the vacancy distribution which allows the ''thermal'' clustering of both the magnetic atoms and magnetic vacancies under specific ''thermal'' conditions. This kind of thermal dilution gives results totally equivalent to those obtained with the usual random dilution method when the order-disorder distribution of the vacancies is obtained away from criticality (*hypercritical* conditions $\theta\gg T_c^{3\mathrm{D}}$) but it gives strongly different results at *critical* conditions ($\theta=T_c^{3\mathrm{D}}$).

In conclusion, our Monte Carlo results in critically thermally diluted (as opposed to randomly diluted) ''grand-canonical'' samples with L increasing show substantial self-averaging improvement of the magnetization in three-dimensional highly diluted ($p=0.5$) Ising ferromagnets.

We gratefully acknowledge financial support from DGCyT through Grant No. PB96-0037.

[1] For a review, see R. B. Stinchcombe, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983), Vol. 7.
[2] A. B. Harris, J. Phys. C **7**, 1671 (1974).
[3] T. C. Lubensky and A. B. Harris, in *Magnetism and Magnetic Materials*, Proceedings of the 20th Annual Conference on Magnetism and Magnetic Materials, San Francisco, 1974, edited by C. D. Graham, G. H. Lander, and J. J. Rhyne, AIP Conf. Proc. No. 24 (AIP, New York, 1975), p. 99; A. B. Harris and T. C. Lubensky, Phys. Rev. Lett. **33**, 1540 (1974).

[4] T. C. Lubensky, Phys. Rev. B **11**, 3573 (1975).
[5] G. Grinstein and A. Luther, Phys. Rev. B **13**, 1329 (1976).
[6] A. Aharony, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6, p. 357.
[7] J. T. Chayes, L. Chayes, D. S. Fisher, and T. Spencer, Phys. Rev. Lett. **57**, 2999 (1986).
[8] W. Kinzel and E. Domany, Phys. Rev. B **23**, 3421 (1981); D. Andelman and A. N. Berker, *ibid.* **29**, 2630 (1984).
[9] S. Wiseman and E. Domany, Phys. Rev. E **52**, 3469 (1995).
[10] A. Aharony and A. B. Harris, Phys. Rev. Lett. **77**, 3700 (1996).
[11] S. Wiseman and E. Domany, Phys. Rev. Lett. **81**, 22 (1998).
[12] F. Pazmandi, R. T. Scalettar, and G. T. Zimanyi, Phys. Rev. Lett. **79**, 5130 (1997).
[13] A. Aharony, A. B. Harris, and S. Wiseman, Phys. Rev. Lett. **81**, 252 (1998).
[14] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989).
[15] S. Wang and R. H. Swendsen, Physica A **167**, 565 (1990).
[16] H. O. Heuer, J. Phys. A **26**, L333 (1993).