Irrelevance of canonical or grand canonical constraints near a random fixed point in large L systems

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The equivalence between canonical and grand canonical constraints near a random fixed point in a critical disordered system is confirmed by means of Monte Carlo simulations. The slow approach to the asymptotic distribution for canonical averaging given by the $L^{(\alpha/\nu)_{random}}$ term is overcome by simulating long range correlated diluted Ising systems with $(\alpha/\nu)_{random}=(a-d)$ for the particular values $a=2$ (linear defects) and $d=3$ (three dimensional systems).

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The critical properties of systems with quenched randomness have been intensively studied during recent decades [1]. One of the most important results is 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, $\alpha_{pure}<0\Rightarrow\nu_{pure}>2/d,\nu_{pure}$ being the correlation length critical exponent of the pure (undiluted) system. This criterion also follows from renormalization group (RG) [3–5], and scaling analyses [6] and it has been extended to the case of strong dilution by Chayes *et al.* [7]. If $\alpha_{pure}>0$ then the system fixed point flows from the pure value toward a new stable fixed point [3–8] at which $\alpha_{random}<0$. A typical example of a system with $\alpha_{pure}>0$ is the three dimensional Ising system. Recently, the Monte Carlo (MC) approach has been used to study the diluted Ising model in two [9], three [10], and four dimensions [11]. The numerical calculations support the existence of a universality class for the randomly diluted three dimensional Ising system different from that of the pure Ising model and independent of the average density of occupied spin states (p). The critical exponents obtained by the MC calculations may be compared with the experimental critical exponents obtained for a random disposition of vacancies in diluted magnets [12].

It is important to take into account that the proof of the Harris criterion by Chayes *et al.* [7] was performed only for the grand canonical constraint (where the average density is fixed, but the actual density has fluctuations of order $N^{-1/2}$, N being the number of sites). It has been recently argued that the proof does not apply in the canonical constraint, where the total number of occupied sites is kept constant and fluctuations are smaller [13]. This means that a proof of the irrelevance of the kind of constraint near a random fixed point is fundamental to establish the validity or not of the Harris criterion for all kinds of disorder.

One way to study if both constraints belong to the same universality class is by means of the lack of self-averaging (SA) given by the value of the normalized squared width in a disordered system at criticality. For a system of linear dimension L and number of sites $N=L^d$, any observable singular property X has different values for different random realizations of the disorder. This means that X behaves as a stochastic variable with average $\overline{X}$ (in the following, the overbar indicates an average over subsequent realizations of the dilution and angular brackets indicate the MC average). The variance would then be $(\Delta X)^2$, and the normalized squared width, correspondingly,

$$R_X=(\Delta X)^2/\overline{X}^2. \tag{1}$$

A system is said to exhibit self-averaging if $R_X\to 0$ as $L\to\infty$ at criticality (with $\xi\gg L$), ξ being the correlation length. The lack of self-averaging is characteristic of random systems with a universality class different from that of the pure model. Two random systems are expected to belong to the same universality class if their values $R_X(\infty)\equiv R_X(L\to\infty)$ coincide. An important question is whether grand canonical and canonical constraints have the same value of $R_X(\infty)$ different from zero or not. This point has been studied recently using a renormalization group analysis in $d=4-\varepsilon$ dimensions, confirming the expectation of a rigorous absence of self-averaging in the three dimensional diluted Ising system for both canonical and grand canonical constraints [14,15]. It follows from the RG analysis that the behavior of the normalized squared width of grand canonical and canonical (C) constraints at criticality turns out to be

$$R_X^{\mathrm{GC}}(L)=R_X(\infty)+A^{\mathrm{GC}}L^{-(\phi/\nu)_{random}}, \tag{2}$$

$$R_X^{C}(L)=R_X(\infty)+A^{C}L^{-(\phi/\nu)_{random}}-B^{C}L^{(\alpha/\nu)_{random}}, \tag{3}$$

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ϕ_{random} being the stability exponent of the random system corresponding to the first correction to scaling and A^{GC},A^{C}, and B^{C} proportionality coefficients depending on the dilution characteristics. Clearly, from the point of view of these RG results $R_X^{\mathrm{GC}}(L\to\infty)=R_X^{C}(L\to\infty)=R_X(\infty)$, indicating that the constraint is always irrelevant, even near the random fixed point.

A value different from zero for the normalized square width of the three dimensional diluted Ising model has also been obtained by MC simulations [10,16,17]. However, the correspondence between the grand canonical and canonical values is much more difficult to check, mainly due to the weak L dependence of the extra term $B^{C}L^{(\alpha/\nu)_{random}}$ appearing when using the canonical constraint [15]. The L dependence given by the stability exponent is not so important since $-(\phi/\nu)_{random}\approx-0.37$ [10]; however, the finite size effects due to $L^{(\alpha/\nu)_{random}}$ are much more important since $(\alpha/\nu)_{random}\approx-0.075$ [10]. Due to this small exponent one might expect the decay to zero near the random fixed point to be extremely slow and inaccessible for present computing facilities, making it impossible to perform the final calculation of $R_X(\infty)$ for the canonical case. Discussion about the application of the $\sqrt{\epsilon}$ series in the study of the short range correlated (SRC) Ising model critical exponents, and in particular of the stability exponent, may be found in Ref. [12].

A possible way to overcome this problem is to use a different way to dilute the system, in particular, to study systems built with long range correlation in the disorder. In all cases previously mentioned, frozen disorder was always produced in a random way, that is, vacancies were distributed throughout the lattice randomly. Real systems, however, can be realized with other kinds of disorder, in which the vacancy locations are correlated. In particular, long range correlation (LRC) in the disorder has been found by means of x-ray and neutron critical scattering experiments in systems undergoing magnetic and structural phase transitions [18,19]. This effect has been modeled by assuming a spatial distribution of critical temperatures obeying a power law $g(x)\sim x^{-a}$ for large separations x [20]. Also, the superfluid transition in liquid ^{4}He has been studied using LRC systems [21,22]. In general, these systems behave in a way very different from that in a randomly diluted system with short range correlation for the vacancy disposition. The basic approach to the critical phenomena of LRC systems was established by Weinrib and Halperin [23] almost two decades ago. They found that the Harris criterion can be extended for these cases, showing that for $a<d$ the disorder is irrelevant if $a\nu_{pure}-2>0$, and that in the case of relevant disorder a different universality class (and a different fixed point) with correlation length exponent $\nu_{random}=2/a$ and specific heat exponent $\alpha_{random}=2(a-d)/a$ appears. In contrast, if $a>d$, the usual Harris criterion for SRC systems is recovered. LRC disorder has been studied also using the Monte Carlo approach for the particular case of a correlation function $g(x)=x^{-a}$ with $a=2$ (defects consisting of randomly oriented lines of magnetic vacancies inside a three dimensional Ising system) [24] and in the case of a (critical) thermal disposition of the vacancies with $a=1.97$ [25,26], confirming in both cases the theoretical predictions of Weinrib and Halperin.

Clearly we would like to be able to answer the following question: what are the values of $L^{-(\phi/\nu)_{random}}$ and $L^{(\alpha/\nu)_{random}}$ in the case of a LRC three dimensional Ising system with $a=2$?

The expected behavior of the first correction to scaling term is an oscillatory one [23]; however, following recent MC results, we may consider $(\phi/\nu)_{random}\approx 1$ with the possible presence of non-negligible higher order corrections [24]. The expected value of the second term in Eq. (3) may be obtained following the Weinrib and Halperin results [23] for the special case of $a=2$ and $d=3$:$(\alpha/\nu)_{random}=(a-d)=-1$.

Clearly, this means that finite size effects are going to be much smaller in the case of a LRC system, making it possible to perform a calculation capable of showing that $R_X^{\mathrm{GC}}(L\to\infty)=R_X^{C}(L\to\infty)=R_X(\infty)$ with today's computing facilities. Following these ideas we now present the numerical calculations we have performed for LRC and SRC Ising systems.

Extensive Monte Carlo simulations have been performed using the three dimensional diluted Ising model for the grand canonical constraint with a dilution probability $p=0.5$ and for the canonical constraint with a fixed value of the concentration of vacancies equal to $c=0.5$. All simulations have been performed for two kinds of disorder. The first kind is the typical SRC system, in which vacancies are distributed throughout the lattice randomly. The second model is an LRC system with randomly oriented lines of vacancies (we should say that there are other ways to construct an LRC system for a given value of a using Gaussian noise [27]). One important fact of our simulations is that the dispersion of concentrations in the grand canonical constraint is taken to be the same in both models (SRC and LRC).

MC calculations have been done for systems with $L=8,16,32$ using 10 000 random realizations and with $L=64$ using 2000 random realizations. To calculate the value of the normalized square width [Eq. 1] we perform calculations of the susceptibility $\chi=\langle M^2\rangle$ per spin for a single value of the temperature using Wolff's single cluster algorithm [28] (cluster algorithms allow a significant decrease in the critical slowing down effect near the critical point [29]). We use 100 000 Monte Carlo steps for equilibration and 500 000 Monte Carlo steps for each calculation. Results are extrapolated to other temperatures using the histogram reweighting method [30]. The critical temperature for each value of L is obtained in an iterative way. From calculations performed at a first trial temperature T_c^a, and using the histogram reweighting method, we obtain $R_\chi(L)$ in a region $T_c^a\pm\Delta T$. Within this region we find a temperature T_c^b where $R_\chi(L)$ has its maximum. T_c^b is then our next trial temperature and we repeat the procedure until both the temperature where calculations are performed and the temperature where the maximum is located coincide within our statistical error. Normally this procedure converges in a few iterations. Using this method we are able to find the value of the normalized

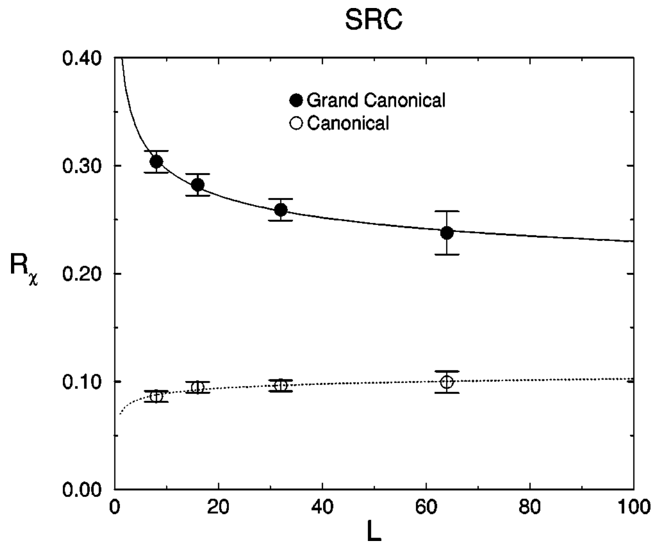

FIG. 1. Normalized square width for the susceptibility (R_χ) vs system's length (L) for canonical (white points) and grand canonical (black points) constraints in the case of a SRC diluted system. Continuous and dotted lines are power law fittings performed for the grand canonical and canonical cases, respectively.

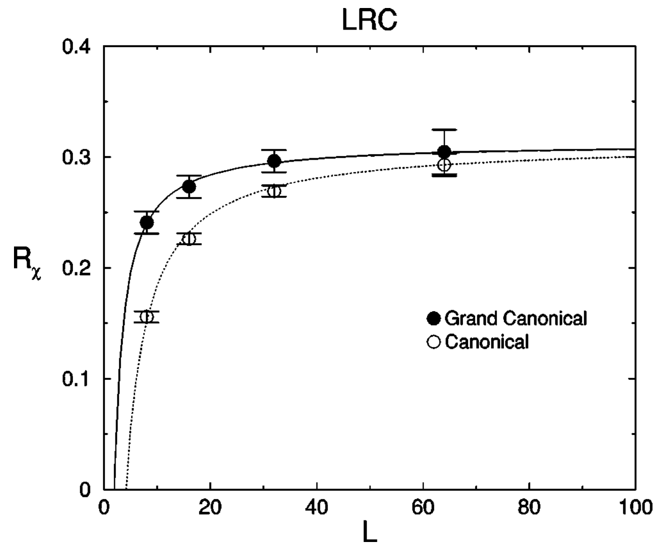

FIG. 2. Normalized square width for the susceptibility (R_χ) vs system's length (L) for canonical (white points) and grand canonical (black points) constraints in the case of a LRC diluted system. Continuous and dotted lines are power law fittings performed for the grand canonical and canonical cases, respectively.

square width and of the critical temperature for each lateral size (L) using both canonical and grand canonical constraints.

Results for SRC systems are presented in Fig. 1. Figure 1 reproduces the kind of behavior previously observed in [15]. The only difference is that now we consider ($p=0.5$, $c=0.5$) instead of ($p=0.6$, $c=0.6$). Clearly, canonical and grand canonical constraints do not merge to the same value of the normalized square width even for L values as great as $L=100$.

The continous line in Fig. 1 is a fitting of the grand canonical numerical data for the SRC case using Eq. (2) with a value for $R_\chi(\infty)$ equal to 0.15 [10]. Canonical data may be fitted using Eq. (3) and the same asymptotic value (see the dotted line on Fig. 1). Note how both fittings are reasonable using the same value of $R_\chi(\infty)$. Since both asymptotic values might be the same, the two constraints might also belong to the same universality class, but clearly it is impossible to detect it directly using the SRC results.

Results for the LRC case are presented in Fig. 2. In this case clearly both constraints have the same value of the normalized square width (R_χ) for $L=64$ within our error bars, indicating that both constraints lead to results belonging to the same universality class.

Again we have performed a fitting to the numerical data using Eq. (2) and Eq. (3) but in this case fixing a value $(\phi/\nu)_{random}=1$ [24] and leaving $R_\chi(\infty)$ as a free parameter. Doing so we obtain a value $R_\chi(\infty)\approx 0.3$, approximately double the one we found for the SRC case.

We may extrapolate our data in Fig. 1 to check the L value needed to obtain a convergence in the SRC results similar to the one obtained in the LRC case (Fig. 2). The L value required is larger than 10^6.

The main difference between the results with canonical and grand canonical constraints comes from the large fluctuations in density existing in the grand canonical case. These fluctuations directly affect the values obtained for the susceptibility at the critical temperature for each realization, resulting in a different finite size behavior. This behavior turns out to be same in the LRC system where the fluctuations in the density have nearly no effect since $-(\phi/\nu)_{random}\approx(\alpha/\nu)_{random}\approx -1$. This equivalence is clearly shown in Fig. 2 where the behavior of canonical and grand canonical constraints is almost the same.

In conclusion, we have used Monte Carlo calculations in systems with long range correlation in the disorder to explicitly confirm the equivalence between canonical and grand canonical constrains. The extremely slow decay to zero of the $L^{(\alpha/\nu)_{random}}$ term existing in systems where the dilution is introduced by a random disposition of the vacancies does not appear in systems with long range correlation in the disorder. In particular, $(\alpha/\nu)_{random}$ equal to -0.075 in the $a=\infty$ case (short range correlated vacancies) turns out to be equal to -1 when using a long range correlated disposition of the vacancies with the particular values $a=2$, $d=3$. This substantial change allows us to confirm explicitly the equivalence between canonical and grand canonical constraints even for L values as small as $L=64$.

The irrelevance obtained in our work is independent of the kind of dilution studied, since the fluctuation $N^{-1/2}$ is an intrinsic property of the grand canonical constraint and has nothing to do with the kind of disordered applied.

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