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Abstract
The renormalization group approach is used to study the effects of a “canonical” constraint (e.g., a fixed number of occupied bonds) on critical quenched disordered systems. The constraint is found to be always irrelevant, even near the “random” fixed point. This proves that $\alpha<0$, or that $\nu>2/d$. “Canonical” and “grand canonical” averages thus belong to the same universality class. Related predictions concerning the universality of non-self-averaging distributions are tested by Monte Carlo simulations of the site-diluted Ising model on the cubic lattice. In this case, the approach to the asymptotic distribution for “canonical” averaging is slow, resulting in effectively smaller fluctuations.

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Critical Disordered Systems with Constraints and the Inequality $\nu > 2/d$

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The critical behavior of systems with quenched randomness has been the subject of much interest for decades. One central issue concerns the correlation length exponent, ν. The so-called Harris criterion [1] showed that the critical behavior of the nonrandom ("pure") system in d dimensions is not sensitive to randomness in the local transition temperature T_c if $\nu_{\rm pure} > 2/d$. The same criterion follows from renormalization group (RG) and scaling arguments [2–5]. When $\nu_{\rm pure} < 2/d$, RG yields a crossover from the pure behavior to a new one, governed by a "random" fixed point. Although the stability of the pure fixed point is determined by the sign of the specific heat exponent $\alpha = 2 - d\nu$, the stability exponent of the random one, $\phi_{\rm random}$, is not related to $\alpha_{\rm random}$ [6], and one has not yet identified any relation between $\alpha_{\rm random}$ and the stability of that fixed point. Independent of these RG arguments, Chayes *et al.* [7] proved that $\nu > 2/d$ even for the case of strong randomness. Their proof considered random binary variables (e.g., the random occupation of bonds or sites), in a "grand canonical" context where the average density is fixed, but the actual density has fluctuations of order $N^{-1/2} = L^{-d/2}$ in a system of linear size L. It has recently been argued [8] that this proof no longer applies for the "canonical" case, when the total number of occupied sites (or bonds) is kept constant. The present Letter investigates the different types of averaging. Although Refs. [7,8] emphasize quantum systems, we feel that the issues under discussion do not depend on that. Therefore, we address them for the simplest case of a random classical ferromagnet. Our new RG analysis shows that the stability exponent for the canonical constraint is always equal to the appropriate value of α. We find that when $\alpha_{\rm pure} < 0$, randomness is irrelevant for both canonical and grand canonical averages. When $\alpha_{\rm pure} > 0$, randomness causes a crossover to the random fixed point. We then show that a positive $\alpha_{\rm random}$ would lead to unacceptable unstable distributions. Thus, we conclude that $\alpha_{\rm random} < 0$, and the random fixed point is stable for both types of averaging. Contrary to the expectation of Ref. [8], our arguments confirm the inequality $\nu > 2/d$ *especially* for the canonical case.

Our second motivation concerns self-averaging in the context of Monte Carlo simulations. Following numerical work and heuristic arguments which indicated the absence of self-averaging [9], it was shown [10] that when a random fixed point is stable, then the distributions of measured quantities $\{X\}$ at the critical point have nonzero relative cumulants, which approach universal values as L increases. This universality was then confirmed by simulations on the grand canonical site-diluted cubic lattice Ising model [9], which found that the relative variances R_χ and R_m (for the susceptibility and the magnetization) reach the same nonzero limiting values for two different site concentrations. However, simulations often use canonical averaging in order to reduce fluctuations [11]. Our new RG results would predict the *same* asymptotic values of R_X, for *both* averages. This is apparently contradicted by new simulations of the above Ising model, presented below, which find that the canonical averaging yields smaller values of R_χ and R_m. However, an important result of the present Letter is that in the canonical case R_X approaches its universal asymptotic value as $L^{\alpha/\nu}$. For the three dimensional (3D) random Ising model, this approach is very slow, and the asymptotic value is not reached for realistic sample sizes. This explains why canonical simulations often observe smaller fluctuations.

It is convenient to perform the RG analysis on a random exchange ferromagnetic spin model: $\mathcal{H} = -2\sum_{\langle ij\rangle} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j$, where $\mathbf{S}_i$ is an m-component unit vector, and $\langle ij\rangle$ indicates summation over pairs of nearest neighbors on a d-dimensional hypercubic lattice. We consider several distributions of the N_b random variables $\{J_{ij}\}$. In the grand canonical case, this distribution is the product of independent factors $P(J_{ij})$, each having an average $J = [J_{ij}]$ and variance $\Delta = [(J - J_{ij})^2]$ (we

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use $[\dots]$ to denote the configurational average). In the extreme canonical case, this product is multiplied by $\delta(\sum_{\langle ij\rangle} J_{ij} - N_b J)$, representing the constraint on the total number of occupied bonds. For example, for bond dilution one has $J_{ij} = J_0$ or 0, with probabilities p and $1 - p$, and the extreme constraint means that the number of occupied bonds in every acceptable realization must be exactly equal to pN_b. A less extreme constraint would arise if we replace $\delta(x)$ by the Gaussian $\exp[-x^2/(2yN_b)]$. As y decreases from ∞ to 0, the "strength" of the constraint increases gradually from the grand canonical limit $y = \infty$ towards the "extreme" canonical limit $y = 0$.

It is also convenient to use the replica method [4,5], and calculate $[Z^n]$, where Z is the realization-dependent partition function and n is the number of replicas, to be sent to zero at the end of the calculation. We next write $Z^n = \mathrm{Tr}\,[\exp(-\beta\mathcal{H}_{\rm eff})]$, with $\mathcal{H}_{\rm eff} = -2\sum_{\langle ij\rangle} J_{ij}\mathcal{E}_{ij}$, where $\mathcal{E}_{ij} = \sum_\alpha \mathbf{S}_i^\alpha \cdot \mathbf{S}_j^\alpha$, and $\{\mathbf{S}_i^\alpha, \alpha = 1,\dots,n\}$ represents the spin in the αth replica. In the grand canonical situation, $[Z^n]$ breaks into a product of independent averages over the N_b different bonds, $[\exp(2\beta J_{ij}\mathcal{E}_{ij})] \equiv \int dJ\, P(J)\exp(2\beta J\mathcal{E}_{ij})$. Expanding in cumulants of $P(J_{ij})$, one ends up with $Z_n \equiv [Z^n] = \mathrm{Tr}\,\exp(-\beta\mathcal{H}_{\rm gr})$, where the trace is over all nm spin components,

$$\mathcal{H}_{\rm gr} = -2\sum_{\langle ij\rangle}(J\mathcal{E}_{ij} + \beta\Delta\mathcal{E}_{ij}^2 + \dots), \qquad (1)$$

and the dots indicate higher cumulants of P, associated with higher powers of $\mathcal{E}_{ij}$. This effective Hamiltonian was the basis for the RG analysis in this "grand canonical ensemble" [4,5,10]. Near the pure fixed point, we can expand the free energy $\mathcal{F}$ to linear order in Δ, which is a measure of the randomness. Since $\langle \mathbf{S}_i^\alpha \cdot \mathbf{S}_j^\alpha\rangle_{\rm pure} \sim t^{1-\alpha_{\rm pure}}$, where $t \sim T - T_c$, the leading correction to $\mathcal{F}$ scales as $N\Delta t^{2(1-\alpha_{\rm pure})}$. Dividing by the leading free energy density, which scales as $Nt^{2-\alpha_{\rm pure}}$, we conclude that Δ appears as $\Delta t^{-\alpha_{\rm pure}}$ [5,12]. It is therefore relevant (irrelevant) when $\alpha_{\rm pure} > 0$ (< 0). When $\alpha_{\rm pure} > 0$, the RG analysis showed a flow towards the random fixed point, which has a finite value of Δ.

In the "canonical ensemble," we include the delta function for the constraint, and use the replacement $\delta(x) = \int d\lambda \exp(i\lambda x)$ [or its generalization $\int d\lambda \exp(i\lambda x - N_b y\lambda^2/2)$]. Repeating the averaging over the individual J_{ij}'s and integrating over λ finally yields

$$\mathcal{H}_{\rm can} = \mathcal{H}_{\rm gr} + (v_0/N_b)\left(\sum_{\langle ij\rangle}\mathcal{E}_{ij}\right)^2 + \dots, \qquad (2)$$

where $v_0 = 2\beta\Delta^2/(\Delta + y)$. The new nonlocal term in $\mathcal{H}_{\rm can}$ is similar to that obtained from constraints in annealed averages, which normally yield the Fisher normalization when $\alpha > 0$ [12,13]. Indeed, once we moved to the replicated space, the random average became "annealed": the final expression for Z_n contains tracing over both the spin and the J degrees of freedom, and in the canonical case the latter trace is constrained. We can now consider the stability of $\mathcal{H}_{\rm gr}$ against the addition of the second term in Eq. (2), which represents the constraint. Each factor $\sum_{\langle ij\rangle}\mathcal{E}_{ij}$ is equal to the total energy of the sample, which scales like $Nt^{1-\alpha}$. Dividing by $\mathcal{F}_{\rm gr} \sim Nt^{2-\alpha}$, we conclude that v_0 scales with $t^{-\alpha}$, just as in the argument presented above [5,12]. However, unlike that argument, the present argument is not restricted to the vicinity of the pure fixed point; v always scales with the exponent α, even near the random fixed point.

This general conclusion is explicitly supported by the RG analysis in $d = 4 - \epsilon$. Here we generalize the calculations of Sak [12] for constraints in compressible magnets. Using Fourier transformed variables, $\mathbf{S}_i^\alpha = N^{-1}\Sigma_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}_i}\boldsymbol{\sigma}^\alpha(\mathbf{q})$, the above two models are both described by a Landau-Ginzburg-Wilson free energy functional of the form

$$\begin{aligned} F = {} & (2N)^{-1}\sum_{\mathbf{q},\alpha}(r + q^2)\boldsymbol{\sigma}^\alpha(\mathbf{q})\cdot\boldsymbol{\sigma}^\alpha(-\mathbf{q}) \\ & + N^{-3}\sum_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}\sum_{\alpha\beta}(u\delta_{\alpha\beta} - w + v\delta_{\mathbf{q}_1,-\mathbf{q}_2}) \\ & \times \boldsymbol{\sigma}^\alpha(\mathbf{q}_1)\cdot\boldsymbol{\sigma}^\alpha(\mathbf{q}_2)\boldsymbol{\sigma}^\beta(\mathbf{q}_3)\cdot\boldsymbol{\sigma}^\beta(-\Sigma_{i=1}^3\mathbf{q}_i) \\ & + \dots, \end{aligned} \qquad (3)$$

where $r \propto (T - [T_c])$, $w \propto \Delta$, and $v \propto v_0$ (the proportionality coefficients involve trivial scale factors [5]), while u represents the usual quartic coefficient of the pure m-vector model. In these equations we have written discrete sums over wave vectors in order to facilitate the proper identification of dependences on $N \equiv L^d$. In the grand canonical limit one has $v = 0$, and the problem reduces to that discussed before [2–5,10]. In the extreme canonical limit ($y = 0$) one has $v = w$. However, the new parameter v appears even for a weak constraint, and therefore one must follow the recursion relations for v together with those for the other parameters.

The RG iterations involve integration over large $\mathbf{q}$, rescaling lengths by factors $e^{-\ell}$, and spins by factors $\zeta = \exp[(d + 2 - \eta)\ell/2]$ [14], so that the renormalized F maintains its form as above [5,15]. To leading order in $\epsilon = 4 - d, u, w$, and v, one has [4,5,12]

$$\begin{aligned} \frac{dr}{d\ell} &= 2r + 4I_1[-(mn + 2)w \\ &\qquad + (m + 2)u + nmv] + \dots, \\ \frac{dv}{d\ell} &= \epsilon v - 4I_2[-2(mn + 2)wv \\ &\qquad + 2(m + 2)uv + nmv^2] + \dots, \\ \frac{dw}{d\ell} &= \epsilon w - 4I_2[-(mn + 8)w^2 \\ &\qquad + 2(m + 2)uw] + \dots, \\ \frac{du}{d\ell} &= \epsilon u - 4I_2[(m + 8)u^2 - 12uw] + \dots, \end{aligned} \qquad (4)$$

with $I_k = K_d/(1 + r)^k$. Note that v does not influence the recursion relations for u and w. Therefore, these remain as they were in the grand canonical case. For $n = 0$

and $m = 1$ one must go to higher order, and the random fixed point becomes of order $\epsilon^{1/2}$ [16,17]. However, all the qualitative features remain the same. Note also that in the limit $n \to 0$, v does not influence the recursion relation for r. This implies that the thermal critical exponents, e.g., ν, are also not affected by the constraint. This is different from the Fisher renormalization that happens for finite values of n. Finally, note that the term of order v^2, and all higher powers of v, disappear from the recursion relation for v when $n \to 0$. We can rewrite the linearized recursion relation for $t = r - r_c$ as $dt/d\ell = t/\nu_{\rm eff} \equiv t\{2 - 4K_d[-2w + (m+2)u] + \ldots\}$. Noting that the same combination of parameters appears in the recursion relation for v, this latter equation can now be written as $dv/d\ell = v\alpha_{\rm eff}/\nu_{\rm eff}$, with $\alpha_{\rm eff} = 2 - d\nu_{\rm eff}$. This agrees with our general scaling argument, and therefore we expect it to remain valid at all orders in the perturbation expansion. We thus conclude that v has only one fixed point value, at $v^* = 0$.

In the extreme canonical case, $y = 0$ and $v = w$. Equation (4) then yields $d(w - v)/d\ell = (\alpha/\nu)_{\rm eff}(w - v) + 16I_2w^2 +$ higher orders. Thus, the initial parameter $w(0) - v(0) = 0$ will increase with ℓ towards positive values, implying an increase in y: the RG maps the initial extreme constraint onto a less extreme one. Note that this equation always prevents $w - v$ from becoming negative. Indeed, a negative value of this difference would imply a negative value of y, which is unstable and unphysical. Beginning in the extreme canonical limit, we expect a few transient iterations, during which $w(\ell) - v(\ell)$ grows from zero to some small finite value C (of order w^2). Near the pure fixed point, both w and v scale with $\alpha_{\rm pure}$, and we have $w(\ell) - v(\ell) \approx C\exp[\ell(\alpha/\nu)_{\rm pure}]$. If $\alpha_{\rm pure} < 0$, the pure fixed point remains stable against both w and v, and they both decay to zero. In contrast, when $\alpha_{\rm pure} > 0$, both w and v flow away from the pure fixed point, and the nonlinear terms in the recursion relations yield an increase of $w - v$. Since the flow of $w(\ell)$ is not affected by v, w still flows towards its random fixed point value $w^*_{\rm random}$, as for the grand canonical case: $w(\ell) \approx w^*_{\rm random} + Ae^{-\ell(\phi/\nu)_{\rm random}}$. However, in the vicinity of that fixed point $v(\ell) \approx Be^{\ell(\alpha/\nu)_{\rm random}}$. If one had $\alpha_{\rm random} > 0$, this would imply a "run away" of $v(\ell)$ towards large positive values, eventually yielding negative values of $w(\ell) - v(\ell)$, which are not allowed. This contradiction implies that we *must* have $\alpha_{\rm random} < 0$, i.e., $\nu_{\rm random} > 2/d$. Indeed, explicit expressions from the ϵ expansion indicate that $-\phi_{\rm random} < \alpha_{\rm random} < 0$ [6]. The same inequality seems also to hold for the 3D random Ising model, where a four-loop calculation with a [3/1] Padé-Borel approximation yields $\phi_{\rm random} \approx 0.245$, while $\alpha_{\rm random} \approx -0.01$ [17]. Since $\alpha_{\rm random}$ has a very small magnitude, one might expect the decay of v towards zero near the random fixed point to be extremely slow. Furthermore, we now expect $v(\ell)$ to first grow, near the pure fixed point, then go through a maximum and then decrease back to zero. The flow is certainly slow near that maximum. In any case, sufficiently close to criticality, and for sufficiently large samples, both the canonical and the grand canonical averages must flow to the same random fixed point, and therefore ratios like R_X must approach the same universal values.

We next calculate R_X for the canonical case, for the example of R_χ. As shown in Ref. [10], $[\Delta X^2]$ and $[X]^2$ have the same renormalization prefactors, and therefore $R_X \equiv [\Delta X^2]/[X^2]$ is invariant under the renormalization group flow. It is thus sufficient to calculate it after ℓ iterations, in terms of $r(\ell), u(\ell), w(\ell)$, and $v(\ell)$. In the replica language, one has $\chi \equiv \langle \boldsymbol{\sigma}^\alpha(0) \cdot \boldsymbol{\sigma}^\alpha(0)\rangle/N$, and $[\Delta\chi^2] \equiv [\chi^2] - [\chi]^2 = \Psi/N^2$, where $\Psi = \langle \sigma_\alpha^2(0)\sigma_\beta^2(0)\rangle$, $\alpha \neq \beta$, and $\langle\rangle$ denotes an average with respect to $\exp(-F)$. We evaluate Ψ diagrammatically, in powers of w and v. It is easy to check that one has

$$\Psi(\ell) = [N(\ell)G(\ell)]^4[N(\ell)]^{-3}[w(\ell) - v(\ell)] + \ldots, \quad (5)$$

where $N(\ell) = N\exp(-d\ell)$, $G(\ell) = 1/[r(\ell) + (e^\ell q)^2]$, with $q \propto 1/L$ representing the smallest wave number allowed in our finite sample, and the dots indicate higher powers of $u(\ell), w(\ell)$, and $v(\ell)$. Similarly, $[\chi(\ell)] = G(\ell)$. Iteration continues until $\ell = \ell^*$, where $G(\ell^*) \sim 1$ [10,15]. The final result, to leading order in $w(\ell^*)$ and $v(\ell^*)$, is

$$R_\chi = [w(\ell^*) - v(\ell^*)]/N(\ell^*). \quad (6)$$

This is exactly of the form found in Ref. [10], except that now $w(\ell^*)$ is replaced by the difference $w(\ell^*) - v(\ell^*)$. Away from criticality ($1 \ll \xi \ll L$), we choose $e^{\ell^*} = \xi$, i.e., $N(\ell^*) = (L/\xi)^d$, and recover strong self-averaging, $R_\chi \sim 1/L^d$. At criticality ($1 \ll L \ll \xi$), we choose $e^{\ell^*} = L$, i.e., $N(\ell^*) = 1$. When the pure fixed point is stable, $\alpha_{\rm pure} < 0$, we find weak self-averaging, $R_\chi \approx CL^{(\alpha/\nu)_{\rm pure}}$, with the amplitude C much smaller than for the grand canonical case. Indeed, it would be very interesting to check this prediction for the canonical averaging in systems with $\alpha_{\rm pure} < 0$ (e.g., the 3D Heisenberg model). When $\alpha_{\rm pure} > 0$, both w and v flow towards the random fixed point. For sufficiently large L and at criticality we expect

$$\begin{aligned} w(\ell^*) &\approx w^*_{\rm random} + AL^{-(\phi/\nu)_{\rm random}}, \\ v(\ell^*) &\approx BL^{(\alpha/\nu)_{\rm random}}. \end{aligned} \quad (7)$$

Thus, R_χ approaches the *same universal value* ($w^*_{\rm random} + \ldots$) for *both* canonical and grand canonical averages in the limit $L \to \infty$. However, in view of the small (negative) value of $\alpha_{\rm random}$, the decay of v to zero may require prohibitively large values of L. In contrast, the approach of w to its fixed point value is relatively rapid [17].

In the simulations [9] three site dilute Ising models were examined, including the two types of disorder. In the grand canonical models each site of the L^3-site cubic lattice was independently either occupied by an Ising spin with probability p or left vacant with probability $(1 - p)$. We used $p = 0.8$ with L up to 64 and $p = 0.6$

with $L \leq 80$. In the canonical model exactly cL^3 sites of each sample were occupied and only the locations of the occupied sites differed between samples. We used $c = 0.6$ with $L \leq 90$. In all models typically thousands of samples were simulated; e.g., at $c = 0.6$, 26 000 (1000) samples for $L = 20(90)$. Simulations were performed at the critical temperatures, $T_c(p = 0.8) = 3.4992$ and $T_c(p = c = 0.6) = 2.4220$, as calculated by Heuer [11], using the Wolff [18] single cluster algorithm [19]. Estimates of critical exponents ratios (such as $\frac{\beta}{\nu}$, $\frac{\alpha}{\nu}$) for the $p = 0.6$ and $c = 0.6$ models were in good agreement with each other. Exponent ratios for $p = 0.8$ agreed well with those of Heuer [11] for a $c = 0.8$ model, in accord with our argument that ν_{eff} is independent of the constraint v.

The relative variances R_m and R_χ are plotted in Fig. 1. First, note that R_X of the grand canonical models, $p = 0.6, 0.8$, seem to approach the same asymptotic values for large L, in agreement with our prediction of universality. However, the canonical ($c = 0.6$) values of R_X remain smaller than their grand canonical counterparts. This difference might suggest a separate universality class for the canonical case, associated with a new fixed point which has $v^* \neq 0$. However, since our RG analysis does not find such a fixed point, we believe that both cases should approach the same asymptotic values, given by the random fixed point values. In spite of this expectation, we note that although the grand canonical value of R_χ, given to leading order by $w(\ell^*)$, may already be very close to w^*_{random} for the L's used in the simulations, the difference between the values of R_χ in the two ensembles is given (to that order) by $v(\ell^*)$. Given Eq. (7), and the smallness of $(\alpha/\nu)_{\text{random}}$, it is reasonable to expect that in the simulations $v(\ell^*)$ has not yet reached its asymptotic value of zero.

In summary, we have considered a quenched randomly diluted Ising model and have shown that, unlike the Fisher renormalization in thermodynamic systems, the canonically and grand canonically quenched random systems are in the same universality class. Their finite size corrections are different because of the appearance of an additional long–ranged potential associated with the global canonical constraint. To avoid RG flows into an unphysical regime, it is necessary to suppose that $\alpha = 2 - d\nu$ is always negative, including at the randomness dominated fixed point. Because the stability exponent for v is α, the flow of v to its fixed point value of zero can be sufficiently slow that it may be difficult to reach the asymptotic regime with numerical simulations.

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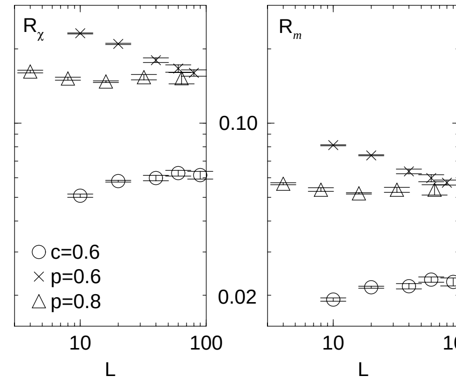

FIG. 1. The relative variances of the susceptibility R_χ (left) and of the magnetization R_m (right) at T_c as a function of L.

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