Critical Behavior of the Specific Heat in the Two Dimensional Site Diluted Ising System

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A Monte Carlo study of the two dimensional randomly site diluted Ising system is reported. The data reveal that the specific heat does not diverge at the critical point, at least when the concentration of dilution is sufficiently large. The critical behavior of the magnetic susceptibility and the correlation length are consistent with pure power-law behavior with concentration dependent critical indices.

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Naive universality arguments would suggest that a randomly site diluted Ising (RSDI) system or a randomly bond disordered Ising (RBDI) system would enjoy the same critical behavior as an undiluted (pure) Ising system. However, a heuristic argument [1] led to the conclusion that the weakest dilution will modify critical behavior if in the undiluted system $\alpha > 0$ (α is the critical index of the specific heat). The 2D Ising model is a marginal case; hence during the years many different opinions have been expressed. The first treatment was initiated by Dotsenko and Dotsenko (DD) [2], who predicted for RBDI $\eta = 0$ and $C_v(t) \sim \ln[\ln(1/t)]$ as $t \to 0$. A different prediction for η was made by Shalaev [3], Shankar [4], and Ludwig [5] who obtained, for the quenched two point function, $[\langle S_{\mathbf{x}} S_{\mathbf{y}} \rangle]_{\rm av} \sim |\mathbf{x} - \mathbf{y}|^{-\eta}$, $\eta = 1/4$, as in the pure case, but they agree with DD on the behavior of $C_v(t)$. All these authors share with DD the key assumption that the continuum limit of the RBDI is the $N = 0$ Gross-Neveu model [6], so they regard the weak disorder in RBDI as a weak four Fermi interaction in the free fermion system, which they treat perturbatively.

At the present time it seems that the generally accepted opinion is that the critical indices are those of the pure Ising model, but modified by logarithmic corrections. Specifically, from the work of Dotsenko and Shalaev (DS) [3], the following generally accepted predictions have emerged:

$$\xi \sim t^{-\nu}[1 + C\ln(1/t)]^{1/2}, \quad \nu = 1,$$
$$\chi \sim t^{-\gamma}[1 + C\ln(1/t)]^{7/8}, \quad \gamma = 7/4,$$
$$C_v \sim t^{-\alpha} \ln[1 + C\ln(1/t)] + C', \quad \alpha = 0. \tag{1}$$

Here $t = (T - T_c)/T_c$, ξ the correlation length, χ the magnetic susceptibility, and C_v the specific heat; the constant C is supposed to be a smooth function of the dilution probability c_i, and should take the same value for all three observables. The logarithmic correction implies a *crossover* of the critical behavior since the logarithmic term dominates in $[1 + C\ln(1/t)]^{1/2}$ when $t \simeq 0$ whereas it is negligible sufficiently far away from a critical point. Accordingly, at temperatures not too close to the critical point the critical behavior of the pure Ising system is expected to be recovered.

Numerical studies for the 2D RBDI [7] claimed that their results confirm DS even for strong disorder; their main observation was $\eta = 1/4$ and $C_v(L, t \doteq 0) \sim \ln[1 + C\ln(L)] + C'$ (L is the linear size of the system), and the latter was regarded as an evidence for Eq. (1). A recent numerical transfer matrix study, however, shows some subtlety, namely, in 2D ν tends to be larger than 1, but the effect is too small to be considered statistically significant [8].

We must mention, however, the one dissenting opinion we are aware of, that of Ziegler [9]: He questions the key assumption of DD, and argues that $N = 0$ Gross-Neveu model is not the continuum limit of the disordered Ising systems but that of the *polymer chains.* One important result of Ziegler's nonperturbative approach is the prediction that $C_v(t)$ does not diverge.

In this Letter we will present the results of an extensive Monte Carlo (MC) study on RSDI (up to $L = 822$ for c_i=1/9, for instance). By measuring the correlation length we could explicitly monitor finite size effects in the MC measurements of the thermodynamic value, unlike any previous numerical work on the subject. We studied c_i = 1/9, 1/4, and 1/3. The statistics of the data are such that a straightforward analysis yields an unambiguous interpretation: For the specific heat, both the thermodynamic data sufficiently close to the critical points and finite size scaling (FSS) data up to $L = 600$ show no indication of diverging behavior for c_i = 1/4 and 1/3. The thermodynamic data of χ and ξ fit to the pure power law (PL) very well with the values of γ and ν increasing with c_i; however, η remains the same as in the pure system. (The main results are summarized in the figures, and the detailed paper including all the numerics will be published elsewhere.)

The Hamitonian of the RSDI is defined as

$$H = \sum_{\mathbf{x},\mathbf{y}} \sigma_{\mathbf{x}} \sigma_{\mathbf{y}} S_{\mathbf{x}} S_{\mathbf{y}}, \tag{2}$$

where $S_{\mathbf{x}}$ is the Ising spin at site $\mathbf{x}$, and $\sigma_{\mathbf{x}}$ takes the

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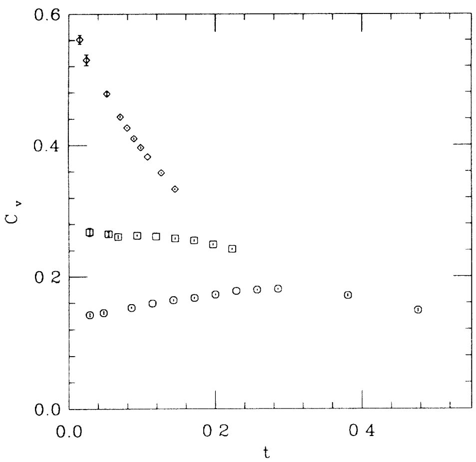

FIG. 1. Thermodynamic value of the specific heat in the scaling regime. The diamond, square, and octagon symbols represent $c_i = 1/9$, $1/4$, and $1/3$, respectively.

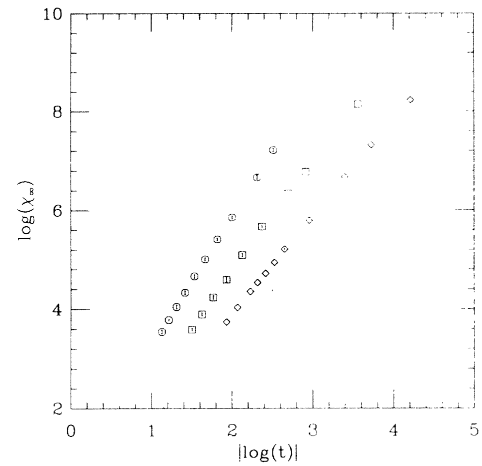

FIG. 2. Thermodynamic data of χ at temperatures such that $\xi_\infty(t) \geq 5$. The slope corresponds to the value of γ. The slope of the dotted line corresponds to $\gamma = 7/4$. One cannot observe any subset of data in the region $|\ln(t)|$ small that exhibit $\gamma = 7/4$, in disagreement with DS scenario. The diamond, square, and octagon symbols represent $c_i = 1/9$, $1/4$, and $1/3$, respectively. For each point of the data with the largest value of $|\ln(t)|$ for $c_i = 1/9$ and $1/4$, $L/\xi_L \geq 10$ is not satisfied, meaning that those values of χ_∞ are slightly underestimated.

values 0 and 1 randomly with probability c_i and $1-c_i$, respectively. Various physical quantities are measured based on the formulas [10] $\chi_L = \sum_{\mathbf{x}} \langle S_0 S_{\mathbf{x}} \rangle$, $\chi' = \sum_{\mathbf{x}} \langle S_0 S_{\mathbf{x}} \rangle e^{2i\pi x_1/L}$, $\xi_L = \sqrt{\chi_L/\chi' - 1}/\sin(2\pi/L)$, and $C_v = \beta^2(\langle H^2 \rangle - \langle H \rangle^2)/2L^2$, where β is the inverse temperature and x_1 represents the first component of $\mathbf{x}$.

The data are obtained by choosing a realization of the dilution process, then running MC in Wolff's one cluster update method [11] with periodic boundary conditions. The procedure is then repeated for several other realizations of the dilution process. Large fluctuations among different realizations are observed as c_i increases, but the average over different realizations converges eventually.

In measuring thermodynamic data, we always choose L so that L/ξ_∞ is fixed for a given c_i: When L/ξ_∞ is sufficiently large the finite size effect will be completely eliminated; otherwise, the quantity is exactly proportional to the corresponding thermodynamic value according to the theory of FSS. We choose $L/\xi_\infty \simeq 20$, 20, and 10 for c_i=1/9, 1/4, and 1/3, respectively [the only exceptions are $\beta = 0.530$ for $c_i = 1/9$ and $\beta = 0.750$ for $c_i = 1/4$, where the corresponding L used are $L = 570$ ($L/\xi_L \simeq 8.35$) and $L = 656$ ($L/\xi_L \simeq 9.24$), respectively], and it turns out that when $L/\xi_\infty \geq 10$ the finite size effect is not significant in measuring the thermodynamic value of C_v. (We chose $L/\xi_\infty \simeq 20$ with the expectation that large value of L/ξ_∞ would reduce the effect of fluctuations among different realizations, but the effect was minimal.)

Sufficiently long thermalization time is important especially for the measurement of C_v with a large L, since the specific heat varies slowly both with temperature and with L. For example, for c_i=1/4 at $\beta = 0.730$ and $L = 660$, we discarded the first 250 000 configurations for the thermalization.

For a given realization of the dilution process, measurements were taken over 10 000–30 000 configurations separated by 3–30 consecutive cluster updatings, and then averaged over different realizations of the dilution process. Usually, the fluctuations due to different realizations were larger than the statistical errors for a given realization of the dilution process. The error estimates associated with these fluctuations were computed with the jackknife method, and in the calculations of χ^2 per degree of freedom (denoted by χ^2/N_{DOF}) we took the total error as twice the error estimate caused by different realizations.

We determined the location of β_c by the crossing of Binder's cumulant ratio method [12]. For $c_i = 1/9$ and $1/4$, β_c was located accurately, while for $c_i = 1/3$ we located only its rough location.

The most remarkable feature of our data comes from the critical behavior of C_v as a function of t (see Fig. 1): While χ_∞ and ξ_∞ are diverging at $t = 0$ (Fig. 2), our data show that $C_v(0)$ is finite for $c_i = 1/4$ and $1/3$ [in fact, $C_v(t)$ is decreasing as $t \to 0$ for $c_i = 1/3$]. This contradicts the DS scenario.

Assuming Eq. (1), the FSS behavior of C_v at the critical point is not obvious. In general, FSS behavior for logarithmic critical behavior cannot be derived in a straightforward way [13], so we do not know how one could obtain $C_v(L, t = 0) \sim \ln[C + \ln(L)] + C'$ from Eq. (1). Our data show that $C_v(L, t = 0)$ is increasing with L very mildly (Fig. 3); one may wonder if this indicates a slow divergence (such as $\ln[\ln(L)]$). We believe that this is not the case. Namely, we observed that for $\beta < \beta_c$, $C_v(L, \beta)$ reaches its thermodynamic value in a nonmonotonic way, first increasing, then decreasing with L to its thermody-

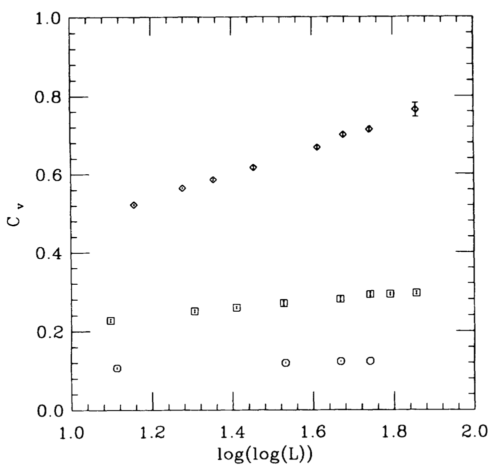

FIG. 3. The FSS of specific heat at the critical points, i.e., β_c=0.5380, 0.772, and 1.11 for c_i=1/9, 1/4, and 1/3. The range of L is $20 \leq L \leq 600$. The diamond, square, and octagon symbols represent $c_i = 1/9$, 1/4, and 1/3, respectively. Note that there is no crossover from $\ln(L)$ to $\ln[\ln(L)]$ behavior for each c_i.

namic value. [In fact at $\beta = 0.530$ the difference between its maximal value and thermodynamic one is about 12% for $c_i = 1/4$ (see Fig. 4).] If we accept FSS [14], according to which $C_v(L,t)/C_v(L = \infty, t)$ is a function of $L/\xi_\infty(t)$ in the scaling regime, then the type of nonmonotonicity observed for $\beta < \beta_c$ would indeed indicate that $C_v(L, t = 0)$ will approach its thermodynamic value from above; moreover, when $C_v(\infty, t = 0)$ is finite, but not very large, the increase of $C_v(L, t = 0)$ must be very mild with L, in agreement with our data for $c_i = 1/4$ and $c_i = 1/3$.

Nondivergent behavior of C_v is consistent with $\nu > 1$ from the rigorous inequality $\alpha \geq 2 - D\nu$ [15] (D is the dimension). Our data of χ_∞ and ξ_∞ are also very consistent with $\nu > 1$, namely, they fit to PL much better than DS as c_i increases. The fitting ranges are sufficiently broad, i.e., $5 \leq \xi_\infty \leq 67$ ([5, 67]), [5, 71], and [5, 48] for $c_i = 1/9$, 1/4, and 1/3, respectively (see Fig. 2 for PL fit). The results are summarized in the following:

(i) $c_i = 1/9$, $\beta_c = 0.5380(3)$. DS: $\chi^2/N_{\rm DOF} \simeq 0.7$, 0.7, and 0.1 for χ, ξ, and C_v, respectively. PL: γ=1.986(10) and ν=1.154(8) with $\chi^2/N_{\rm DOF} \simeq 0.8$ and 0.9, respectively.

(ii) c_i=1/4, $\beta_c = 0.772(1)$. DS: $\chi^2/N_{\rm DOF} \simeq 5.0$, 4.1, and 3.0 for χ, ξ, and C_v, respectively. PL: $\gamma = 2.244(26)$ and $\nu = 1.306(19)$ with $\chi^2/N_{\rm DOF} \simeq 2.4$ and 2.6, respectively.

(iii) $c_i = 1/3$, $\beta_c = 1.10 \sim 1.11$. DS: $\chi^2/N_{\rm DOF} \simeq$ 3.6[7.4] for χ, assuming $\beta_c = 1.10[1.11]$. PL: $\gamma = 2.49(5)[2.64(8)]$ and $\nu = 1.49(3)[1.57(5)]$ with $\chi^2/N_{\rm DOF} \simeq 0.25[0.10]$ for χ, assuming $\beta_c = 1.10[1.11]$

For c_i=1/4 and 1/3, the DS fitting is extremely unstable in the parameter space and the value of C tends to be very large [in other words, the minimum of χ^2 is highly

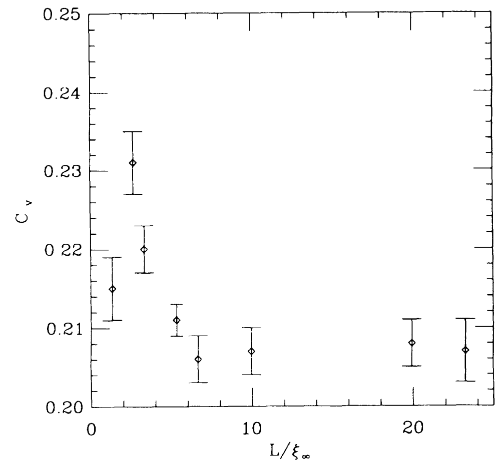

FIG. 4. Specific heat as a function of L/ξ_∞ at $\beta = 0.530$ for $c_i = 1/4$.

insensitive to the change of C, for example, even from $C = O(10^4)$ to $C = O(10^5)$ for $c_i = 1/4$], which means that the fitting is basically poor; also, the comparison of $\chi^2/N_{\rm DOF}$ definitely favors PL over DS.

Note that the pure PL fits yield $\eta \equiv 2 - \gamma/\nu \simeq 0.25$ for all c_i; the situation is very similar with the critical behavior of the Ashkin-Teller model [16], where there exists a critical line (in the space of coupling constants) along which critical indices such as γ, ν, and α are continuously changing while $\eta = 1/4$ remains fixed [17]. This model has served as a salient example suggesting that universality classes are characterized by the value of η instead of ν or γ. In RSDI, the concentration of dilution does not change the symmetry of the Hamiltonian so η remains the same, but other critical exponents change. Our FSS data at a critical point from $L = 20$ to $L = 600$ also confirm $\eta = 1/4$ (see Fig. 5); it is clear that $\chi_L \sim L^{\gamma/\nu}$

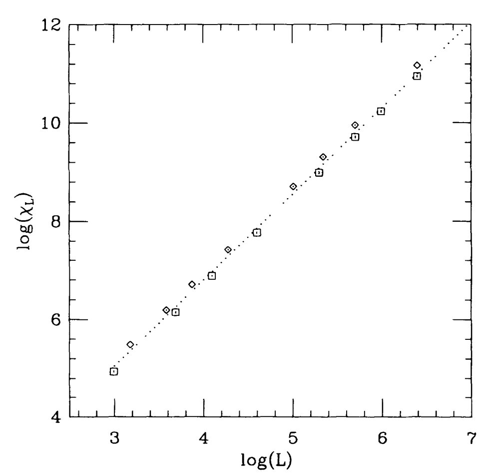

FIG. 5. FSS data of χ at the critical point for $c_i = 1/9$ and 1/4. The slope gives γ/ν and the slope of the dotted line corresponds to $\gamma/\nu = 7/4$. The diamond and square symbols represent $c_i = 1/9$ and 1/4, respectively.

and $\gamma/\nu = 1.76(1)$ for $c_i = 1/9$ and $1/4$.

For $c_i = 1/9$, neither thermodynamic nor FSS data give a clear indication which fit is better. Although much more extensive MC simulation might be required for the clarification, we believe that even for the weakest dilution DS type critical behavior is not plausible: We notice that Binder's cumulant ratio at the critical point $[U_L(\beta_c]$ is increasing with c_i [18] $[U_L(\beta_c) = 1.832(2), 1.85(1), 1.87(1),$ and $1.90(2)$ for $c_i = 0, 1/9, 1/4$, and $1/3$, respectively] as it does with ν along the critical line of the Ashkin-Teller model [19]. In addition, it was not possible to observe any indication of a crossover in the scaling region which the DS fit predicts; to be more specific, a scaling region displaying the critical behavior of the pure Ising system could not be observed (see Figs. 1–3).

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