

The critical behavior of three dimensional Heisenberg models on disordered lattices: Possible violation of Harris criterion in diluted magnetic semiconductors

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Using direct Monte Carlo simulation, we calculate critical exponents for disordered Heisenberg models on a three dimensional lattice with deleted sites (as in nearest neighbor simple cubic models or dilute magnetic semiconductors) or missing bonds, finding substantial shifts in the critical exponents (and hence the universality class) even for weak disorder. Our calculations indicate the change in critical behavior (e.g. as manifested in substantial shifts in the correlation length exponent ν) to be directly related to the disorder strength as parameterized by the percentage of missing moments or bonds. Our work indicates a strong violation of the Harris criterion in diluted magnetic semiconductors.

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A question of great fundamental importance is the relationship between the critical properties of a pure magnetic system with its disordered counterpart, i.e. the extent to which critical properties are universal with respect to disorder in the system. In this letter we theoretically address this question for the 3D disordered cubic Heisenberg model, finding the unexpected answer that disorder, even when it is relatively weak, could modify the critical exponents.

Technologically relevant magnetic materials such as dilute magnetic semiconductors (DMS) are characteristically strongly disordered due to the low concentration of magnetic moments (e.g. $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ where 5% - 12% of the Ga sites are occupied by substituent Mn ions). DMS materials such as $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ have been modeled theoretically via a Heisenberg model on an fcc lattice where the Hamiltonian is $\mathcal{H} = \sum_{ij} J(r_{ij})\mathbf{S}_i \cdot \mathbf{S}_j$ with $J(r_{ij})$ being a carrier (hole) mediated indirect exchange damped RKKY coupling between moments separated by a distance r_{ij} given by $J(r) = J_0 e^{-r/l} r^{-4} [\sin(2k_F r) - 2k_F r \cos(2k_F r)]$. $k_F = (\frac{3}{2}\pi^2 n_c)^{1/3}$ is the Fermi wave number, n_c is the hole density, and l is the damping scale. While specific parameters such as the ferromagnetic transition temperature T_c have been calculated in theoretical studies [1, 2], the critical behavior of disordered Heisenberg models on a three dimensional lattice has not been understood in detail. At the ferromagnetic transition, thermodynamic quantities scale as power laws in the reduced temperature, $t = (T - T_c)/T_c$ with, e.g., the magnetization varying as $m \propto t^\beta$ and the correlation length scaling as $\xi \propto t^{-\nu}$, and hence critical exponents such as β and ν (up to material specific prefactors) completely specify the critical behavior near T_c where $t \ll 1$.

Our task is to determine the extent to which the critical behavior of the three dimensional Heisenberg model is influenced by disorder. A theoretical result (derived from a renormalization group calculation) known as the

Harris criterion [3] holds that the sign of the specific heat exponent α determines whether the critical exponents are altered. Specifically, although modifications in the universality class are expected for $\alpha > 0$, the Harris criterion predicts that disorder will not affect the critical exponents when $\alpha < 0$. The hyper-scaling identity $\alpha = 2 - d\nu$ implies that the condition for stable critical behavior is $\nu > 2/d$, $d = 3$ being the dimensionality of our system. In particular, since $\nu = .7 > .67$ for the Heisenberg model [4], the Harris result precludes disorder induced shifts in the critical exponents. Nevertheless, we have found via direct large-scale Monte Carlo calculations that the critical behavior is modified with ν ranging from ~ 0.725 to ~ 0.76 for site diluted simple cubic models with similar deviations ($\nu = 0.77 \pm 0.03$) for damped RKKY models for DMS. The experimental DMS materials are therefore likely to violate the Harris criterion.

Another component of the Harris criterion is the prediction that thermodynamic variables such as the magnetization and magnetic susceptibility do (do not) self-average at T_c in the bulk limit when $\nu > (<) 2/3$. The extent of self-averaging may be quantified via the parameter $g_2 = ([\langle m^2 \rangle^2] - [\langle m \rangle]^2)/[\langle m^2 \rangle]^2$ [5], the relative variance of $[\langle m^2 \rangle]$ with respect to disorder where m is the magnetization, angular brackets indicate thermal averages, and square brackets refer to disorder averaging.

In this letter we show via a large-scale Monte Carlo study that the critical exponents are not fixed, but instead vary continuously with increasing disorder strength, changing substantially even for weak disorder. Using detailed Monte Carlo studies of g_2 , we find self averaging to be intact when interactions between magnetic moments are exclusively ferromagnetic. We calculate g_2 with sufficient precision to quantitatively corroborate the disorder induced shifts we find in the critical exponents. To carefully examine a broad range of disorder, our most detailed results are obtained for the case of the diluted

simple cubic Heisenberg model with nearest neighbor interactions between spins where c is the magnetic moment concentration giving the percentage of occupied sites. We examine many values of c , from $c = 0.95$ where disorder is quite weak to $c = 0.4$ in the vicinity of the site percolation threshold $c_p = .3116$ [6], where critical exponents seem to converge to a strong disorder limit. Though DMS materials (e.g. with much lower magnetic ion concentrations) differ in many ways from the nearest neighbor simple cubic model even when the latter is in the strong disorder regime near the percolation threshold, in both cases our calculations yield similar results for the critical behavior, showing no change in β/ν but on the order of a 10% increase in ν .

Singularities in variables such as the specific heat and magnetic susceptibility are smoothed as $t \rightarrow 0$ and the correlation length ξ becomes comparable to the system size L . However, we can determine critical exponents by exploiting finite size scaling at T_c ; the magnetization scales as $m \propto L^{-\beta/\nu}$ while the thermal derivative $d\xi/dT$ varies as $d\xi/dT \propto L^{1/\nu}$, and one obtains exponents ν and β/ν by calculating m and $d\xi/dT$ for many different system sizes and carefully extrapolating to the thermodynamic limit. ν and β/ν are sufficient to calculate additional exponents (e.g. α for the specific heat and γ for the magnetic susceptibility).

To obtain critical exponents accurately, it is essential that calculations be performed as close as possible to T_c [7] since the temperature range where finite size scaling holds narrows with increasing L . To obtain T_c as precisely as possible, we numerically calculate the normalized correlation length ξ/L following reference [8]. For temperatures below T_c , ξ/L ultimately increases with increasing L , while above the Curie temperature, ξ/L eventually decreases. We find T_c by insisting that ξ/L tend to a constant value for very large system sizes (e.g. containing 10^7 spins) where finite size effects are negligible. Alternatively, we also examine the Binder cumulant $U_4 = 1 - [\langle m^4 \rangle] / 3[\langle m^2 \rangle]^2$. In this manner, we calculate T_c to within one part in 10^4 . In addition to facilitating the calculation of T_c , the Binder cumulant can also be used to determine ν since dU_4/dT and $d\xi/dT$ both scale as $L^{1/\nu}$ at T_c .

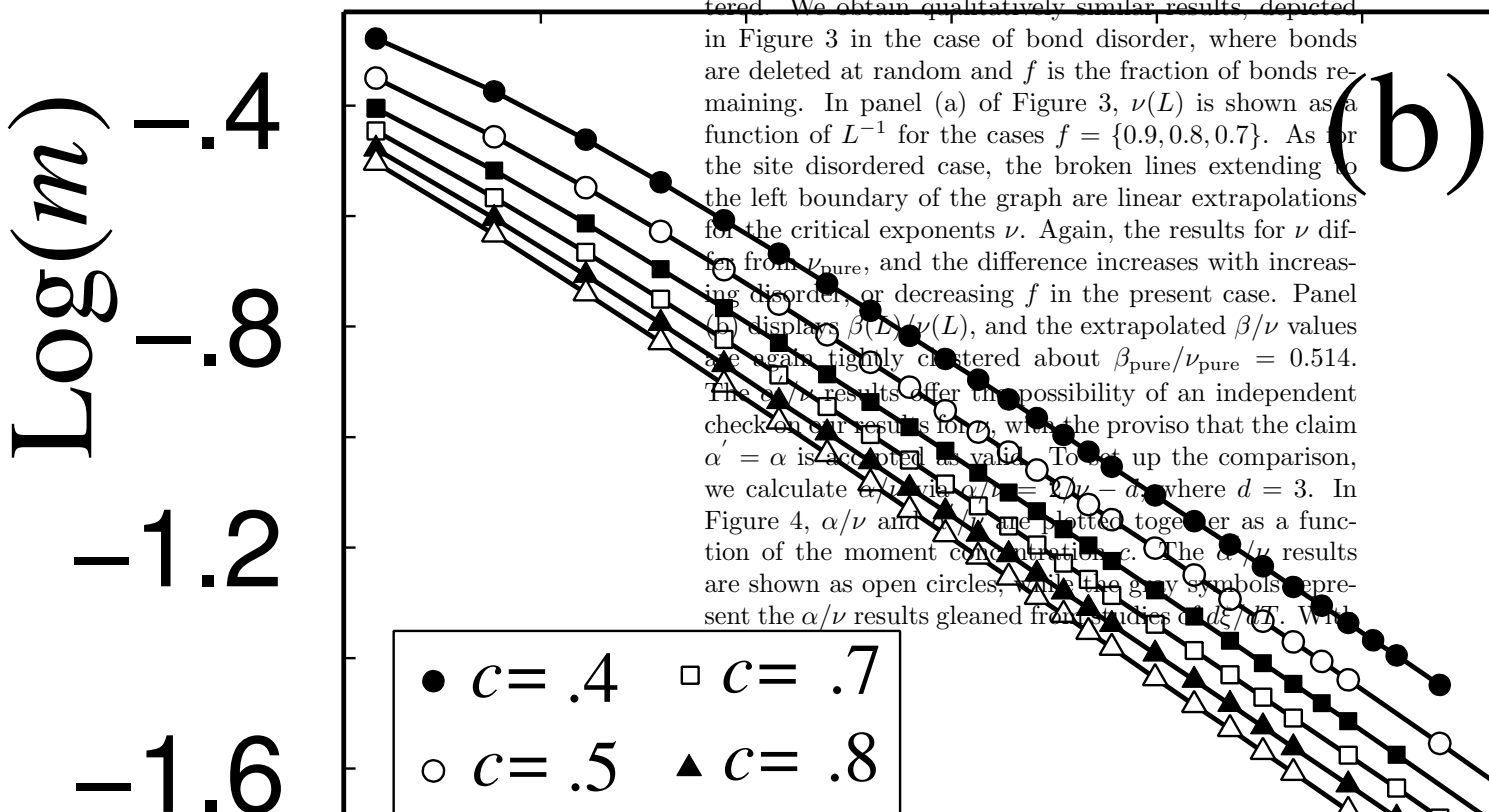
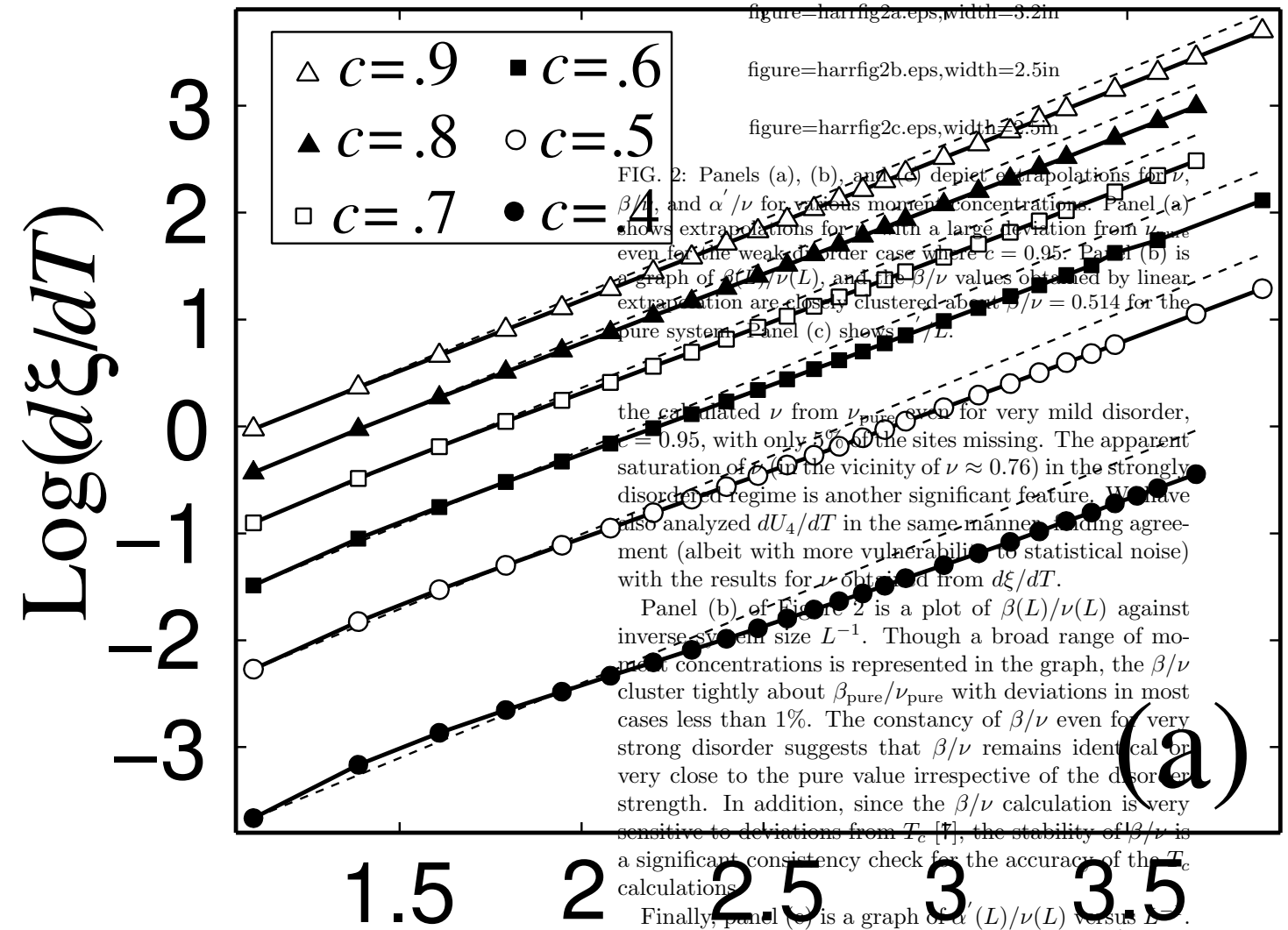
The calculation of critical exponents involves the exploitation of finite size scaling trends easily obscured by statistical fluctuations stemming from the random character of the disorder and hence it is necessary to average over many realizations of disorder, 10^5 for $c < 0.9$ and at least 4×10^4 for weak disorder where $c = 0.9$ and $c = 0.95$. To circumvent critical slowing down which plagues local update techniques such as the Metropolis method, our Monte Carlo calculations employ cluster updates to flip large sets of correlated spins. Specifically, we use alternating Wolff cluster [9] and Swendsen-Wang sweeps [10], the latter being included because the Swendsen-Wang steps address every spin, including isolated clusters of

moments inaccessible to Wolff cluster moves. To reduce the severity of finite size effects, we examine cubic systems of size L with periodic boundary conditions. We use 1000 hybrid sweeps per disorder realization, and equilibration effects are eliminated by discarding the first quarter of the Monte Carlo sweeps. Thermal derivatives such as $d\xi/dT$ and dU_4/dT need not be calculated via numerical differentiation; it is more convenient instead to use $d\langle q \rangle/dT = (\langle qE \rangle - \langle q \rangle \langle E \rangle) / (k_B T^2)$ obtained by direct differentiation of $\langle q \rangle = \sum_{\text{conf}} q_{\text{conf}} \exp(-E_{\text{conf}}/k_B T) / Z$, where the sum is over all possible system configurations, Z is the partition function, E is the internal energy, and q is a generic thermodynamic variable such as the magnetization.

Asymptotic finite size scaling behavior such as $m \propto L^{-\beta/\nu}$ and $d\xi/dT \propto L^{1/\nu}$ implies the corresponding log-log plots will become linear for large enough L with the slope yielding the critical exponent of interest. Figure 1 shows log-log plots of $d\xi/dT$, m , and g_2 . Panel (a) of Figure 1 depicts $d\xi/dT$; the broken lines with slope $1/\nu_{\text{pure}}$ are included to highlight deviations of the $d\xi/dT$ curves from the pure case with the differences in slope increasing with decreasing c . In panel (b), the magnetization curves make a smooth transition to linear behavior. On the other hand, the log-log g_2 curves in panel (c) of Figure 1 are non-monotonic, increasing for small values of L and attaining a maximum (typically for systems containing on the order of 700 spins) before decreasing and ultimately becoming linear for sufficiently large system sizes. The non-monotonic behavior in g_2 also occurs for bond disordered systems as well as damped RKKY models for DMS and appears to be a generic feature of disordered Heisenberg models. A power law decay in L of g_2 for large system sizes is consistent with a monotonic decrease of g_2 , a hallmark of self-averaging in the bulk limit. It has been argued that g_2 scales as $L^{-\alpha/\nu}$ [11] and, as we discuss later, our results support the identification of α' with the specific heat exponent α .

Scaling behavior such as $d\xi/dT \propto L^{1/\nu}$ suggests that critical exponents might be obtained by comparing systems of different sizes; e.g., for the pair $(L, 2L)$, ν would be obtained with $\nu = \ln(2) / [\ln(d\xi/dT|_{2L}) - \ln(d\xi/dT|_L)]$. However, the results are influenced by finite size effects, and exponents obtained in this manner are more appropriately regarded as “local” L dependent exponents $\nu(L)$, $\beta(L)/\nu(L)$, and $\alpha'(L)/\nu(L)$. It is important to carefully extrapolate to the thermodynamic limit by examining a broad range of system sizes. We consider systems with as few as 20 spins to larger systems with on the order of 10^5 moments.

Figure 2 contains graphs of $\nu(L)$, $\beta(L)/\nu(L)$, and $\alpha'(L)/\nu(L)$ as a function of L^{-1} . Panel (a) of Figure 2 shows $\nu(L)$ as a function of inverse system size L^{-1} . The broken lines connecting the curves to the left boundary of the graph are linear extrapolations to the bulk limit where $L^{-1} = 0$. There is a substantial deviation of



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FIG. 3: The graphs are extrapolations for critical exponents for bond disorder. Panel (a) is a graph of $\nu(L)$ versus L^{-1} . The variable f indicates the fraction of bonds present. The lower boundary of the plot coincides with $\nu_{\text{pure}} = .698$. Panel (b) depicts $\beta(L)/\nu(L)$, with the broken line indicating β/ν for the pure case. The linearly extrapolated β/ν ratios for all three values of f are within 1% of $\nu_{\text{pure}} = .514$.

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FIG. 4: The main graph is a plot of the ratio α/ν (gray symbols) and α'/ν (open symbols), the finite size scaling exponent for the self-averaging parameter g_2 . The plot shows reasonable agreement between the α/ν and α'/ν values when the error bars are taken into account. The inset shows T_c from the site percolation threshold $c = .3116$ to the pure model with $c = 1$.

the exception of the case $c = 0.4$, where the discrepancy may be due to systematic effects introduced in the extrapolation to the bulk limit, the α'/ν and α/ν data are in agreement within the bounds of Monte Carlo error, shown as error bars which overlap for $c > 0.4$. Figure 5 shows results for the damped RKKY model [1, 2] for $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ where $x = .05$, $n_c/n_i = .1$, and $l/a = 0.5$, a being the fcc lattice constant. In this strongly disordered situation, we find β/ν to be close to the pure value as in the bond and site disordered nearest neighbor models, and we again find $\nu = 0.77 \pm 0.03$ to be much higher than its pure Heisenberg model counterpart. Using $\alpha = 2 - d\nu$, we obtain $\alpha/\nu = -0.40 \pm 0.07$, compatible to within Monte Carlo error with the independently calculated $\alpha'/\nu = -0.45 \pm 0.075$.

In conclusion, we have examined Heisenberg models on disordered three dimensional lattices for both site and bond disorder, finding bulk self-averaging to be intact as predicted by the Harris criterion. On the other hand, our finite size scaling studies show that the critical exponents vary with the strength of the disorder in contrast both to the Harris criterion prediction of stable critical exponents and indications of a single random fixed point for the case $\alpha > 0$ (e.g. for the site diluted Ising model) [12]. We

find that while shifts in critical behavior set in rapidly as disorder is introduced, the critical exponents saturate for

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FIG. 5: Critical exponent extrapolation graphs for DMS; $l/a = 0.5$, $x = 0.05$, and $n_c/n_i = 0.1$. Panels (a), (b), and (c) are extrapolation graphs for ν , β/ν , and α' respectively; panel (d) is a log-log plot of the self-averaging parameter g_2 . The gray error bars indicate the possible range for the extrapolated exponents.

moderate to strong disorder (e.g. $c \geq 0.7$ for the case of site disorder) with ν ultimately increasing by 10%. For the very strongly disordered magnetic semiconductors, we also find significant increases in ν with, e.g., $\nu = 0.77$ for $l/a = 0.5$, $x = 0.05$, and $n_c/n_i = 0.1$. We speculate that the rapid change of ν for weak disorder is a signature of non-analytic behavior (i.e. a diverging $d\nu/dc$) in the weak disorder $c = 1$ limit, a phenomenon difficult to capture with perturbative treatments.

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