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COMMENT

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Abstract. We use Monte Carlo simulations to estimate for the first time the corner critical exponents for the three-dimensional Ising model with free boundary condition at bulk criticality. Finite-size dependences of the spin-spin correlation functions are used to obtain $\eta_{\text{bulk-corner}} = 1.75 \pm 0.2$.

Critical phenomena of systems with free boundaries have attracted much interest in recent years. Critical properties of three-dimensional systems possessing free surfaces (Binder 1983, Zia 1984, Jasnow 1987 and Diehl 1987) and edges (Cardy 1983, Mon and Valles 1989, Privman 1988) have been investigated both analytically and numerically and the corresponding critical exponents for surface (Binder 1983, Binder and Landau 1984) and edge (Cardy 1983) transitions were computed analytically and consistent with Monte Carlo simulations (Binder 1983, Binder and Landau 1984, Mon and Valles 1989). There have also been some studies of two-dimensional (Cardy and Peschel 1988) critical systems possessing a free corner using conformal algebra. In contrast, results for the free corners in three dimensions have been more limited. In three dimensions, finite-size scaling arguments (Privman 1989) indicate a logarithmic finite-size dependence term in the corner free energy and recent Monte Carlo results (Lai and Mon 1989) are consistent with the predictions. Critical exponents describing corner spins have not yet been reported.

In general, the spin-spin correlation function $g(\boldsymbol{r})$ at criticality has a power law decay which in the larger r limit has the form

$$g(\boldsymbol{r}) \sim r^{-(d-2+\eta)} \tag{1}$$

where d is the spatial dimension and η is the related correlation function decay exponent. In this comment, we use Monte Carlo simulation to estimate the exponents η_{03} and η_{33} by studying the correlation functions g_{03} and g_{33} on a L^d lattice with free boundary conditions. The subscripts 0 and 3 represent the bulk and corner spins respectively. This technique has been shown to be very useful for estimating surface critical exponents (Nightingale and Blöte 1988).

The nearest-neighbour ferromagnetic Ising model is simulated on a simple cubic lattice with free boundary conditions at bulk criticality. The correlation function g_{03} (at maximum separation) is given by

$$g_{03}(\sqrt{3}L/2) = \langle s_0 s_3 \rangle - \langle s_0 \rangle \langle s_3 \rangle \tag{2}$$

where the spin in the bulk s_0 is taken to be at the centre of the lattice and s_3 is a spin at a corner. The $\langle\ \rangle$ represents the ensemble average. g_{03} satisfies the scaling relation

$$g_{03} \sim L^{-(1+\eta_{03})}. \tag{3}$$

The correlations among the corner spins $g_{33}(L)$ are computed similarly. The surface couplings are the same as the bulk and take the critical value 0.221 654 (Pawley *et al* 1984) in units of $k_B T$. The standard spin-flip Monte Carlo method is employed for $3 \leqslant L \leqslant 17$ up to 10^7 Monte Carlo steps per spin. Statistical uncertainties are estimated by different runs, typically about four to six. Figure 1 is a log-log plot of $g_{03}(\sqrt{3}\, L/2)$ against L. The data can be fitted well by a straight line over the range of sizes considered. A least squares fit for all data gives $\eta_{03} \simeq 1.76 \pm 0.2$ while the data for $L \geqslant 7$ give $\eta_{03} \simeq 1.75 \pm 0.2$. We also estimated η_{33} by evaluating $g_{33}(L)$, which decreases much fast and requires much more statistics. The results for large lattice sizes are not accurate even with long runs. From our data for $L \leqslant 11$, η_{33} is roughly estimated to be $\simeq 3.3 \pm 0.4$ (see figure 2). If one assumes the general scaling relation (Cardy 1983)

$$\eta_{pq} = \tfrac{1}{2}(\eta_{pp} + \eta_{qq}) \tag{4}$$

to also hold for the case involving the corners, then using the known (Liu and Fisher 1989) value of $\eta_{00} \simeq 0.0388$ and our estimated value of η_{03}, then η_{33} is predicted to be 3.46 ± 0.3. This is consistent with our simulation estimate. Thus our result agrees with the general relation (4) within the statistical errors for the Ising model with free corners in three dimensions. Although the range of sizes considered here is not impressive, nevertheless our data scale very well. Further simulations will be in order if these results can stimulate analytical studies of corner exponents.

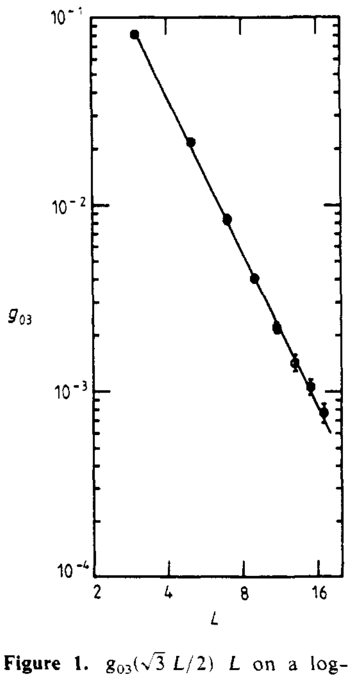

Figure 1. $g_{03}(\sqrt{3}\, L/2)$ L on a log-log plot. The straight line is a linear least squares fit for $L \geqslant 7$.

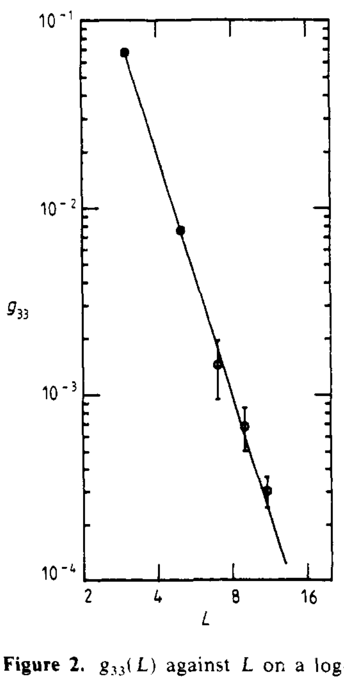

Figure 2. $g_{33}(L)$ against L on a log-log plot. The straight line is a linear least squares fit for $L \leqslant 11$.

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