Critical and Topological Properties of Cluster Boundaries in the 3D Ising Model

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We analyze the ensemble of surfaces surrounding critical clusters at $T = T_c$ in the 3D Ising model. We find that $N_g(A)$, the number of surfaces of genus g and area A, behaves as $A^{x(g)}e^{-\mu A}$. We show that μ is constant and $x(g)$ is approximately linear; the sum $\sum_{g} N_g(A)$ scales as a power of A. The cluster volume is proportional to its surface area. We discuss similar results for the ordinary spin clusters of the 3D Ising model and for 3D bond percolation.

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It is a long-standing hope in theoretical physics that it is possible to find a formulation of three-dimensional phase transitions dual to the usual order parameter field theory. Such a description recasts the dynamics in terms of fluctuating surfaces. In the 3D Ising model such a reformulation is indeed possible on the lattice [1], and the relevant problem is the existence of a continuum limit for the surface theory. Despite much theoretical effort, real progress in this direction has been slow and difficult. In order to provide some experimental data to perhaps point in the right direction, we embarked on a numerical study of surfaces in the 3D Ising model.

The main obstacle to a continuum description of free random surfaces is the well-known fingering instability of surfaces in embedding space of dimension $d > 2$ [2]. One motivation for our study was to see if the fingering instability plagues Ising surfaces, to see if their natural mutual avoidance stabilizes the fingering instability. In fact, one could regard our investigations purely as a study of ensembles of self-avoiding random surfaces, with the Ising model as a convenient tool for generating them [3,4]. We searched for scaling properties in the distribution of surfaces of fixed genus, to see if a scaling limit could exist. We will present data that show nontrivial topologydependent scaling behavior for self-avoiding surfaces in 3D (for previous work, see [5]).

Contrary to the widely held belief that a phase transition is characterized by nested clusters of ordered domains of all possible sizes, it has been shown [6] that the distribution of domain boundaries in the 3D Ising model does not scale at criticality. Rather, as the critical point is approached from low temperatures, islands of flipped spins (which we shall call minority clusters) merge into

a large percolating cluster at a temperature T_p well below the critical temperature T_c . The dynamics is then dominated not by the entropy in the cluster distribution but by the entropy of configurations of the percolating cluster. Moreover, no local order parameter of the Ising model reflects this percolation transition.

However, there exists a cluster representation of the Ising model due to Fortuin and Kasteleyn (FK) [7] which captures the critical properties of the model, in particular that the divergence of the correlation length is related to the percolation of the FK clusters. These clusters are formed by adjoining neighboring spins with a probability $1 - e^{-2\beta}$ if they are equal. The FK representation led Swendsen and Wang (SW) to propose a Monte Carlo algorithm that partially defeats critical slowing down [8]. In our simulations we have used the SW algorithm. We studied the self-avoiding surfaces bounding both minority spin clusters (at T_p) and FK clusters (at T_c). To explore further the possible realizations of self-avoidance, we also simulated the surfaces defined by pure bond percolation [9]. It should be emphasized that the "bosonic" surfaces defined by Ising domain walls are not the same as the "fermionic" surfaces that arise in the surface reformulation of the lattice Ising model; nevertheless, we expect that they should capture the characteristic features of any critical surface theory of the 3D Ising model.

We ran a medium sized simulation, using roughly four months of time on RISC workstations. We have analyzed Ising configurations on a $64³$ body centered cubic (bcc) lattice at the Curie temperature, $\beta_C = 0.0857$, using 0.3×10^6 iterations. We also collected data on simple cubic lattices of size 32^3 and 64^3 at the Curie temperature, $\beta_C = 0.221651$ (performing about 6×10^6 and 0.25×10^6 iterations, respectively). Data were also taken at the minority percolation point β_p for the Ising model (where we also studied many different lattice sizes, going from $32³$ to $100³$) and for pure bond percolation on the simple cubic lattice. All of our error analysis has been done by using jack-knife and binning techniques. For more details see Ref. [10].

On the bcc lattice, we coupled with equal strength both the six nearest and eight next-nearest Ising spins so that only three plaquettes of the dual lattice meet along a dual link. Since surfaces built this way on the bcc lattice are naturally self-avoiding, computing the genus of the dual surface is trivial. The number of handles q is obtained through the Euler formula $2 - 2g = V - L + P$, where $V, L,$ and P are the number of vertices, links, and plaquettes, respectively, on the dual surface. On the other hand, the genus definition on the simple cubic lattice is more problematic, and requires a few choices (which we discuss in detail in Ref. [10]) to resolve ambiguities where surfaces self-touch.

Overall, for the FK clusters we obtained our best results on the bcc lattice. We found a scaling law for the number of clusters of volume V_{cl} , $N(V_{\text{cl}}) \sim V_{\text{cl}}^{-\tau}$; the exponent $\tau = 2.22$ [11] with a large systematic error which could be as high as 3% [10]. We also measured the quantity $A_{\rm cl}$, which counts the number of cluster sites on the boundary, and found that asymptotically it was proportional to the cluster volume V_{cl} .

Figure 1 shows this dependence on the simple cubic lattice. We see that for very small volumes, the lattice regularization constrains V_{cl} to equal A_{cl} and for intermediate volumes, there is a small deviation from linear scal-

 0.08 0.06 $\begin{array}{l} \ln(V_{\rm el}/A_{\rm el}) \\ 0.04 \end{array}$ 0.02 \circ 10 6 8 $ln(V_{cl})$: cluster volume (L=64 SC, 3d lsing FK clusters)

FIG. 1. $\ln(V_{\text{cl}}/A_{\text{cl}})$ vs $\ln(V_{\text{cl}})$ for FK clusters on the $L = 64$ simple cubic lattice.

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ing (as some interior sites begin to appear). The plateau that appears around $V_{\text{cl}} = 3000$ indicates the onset of scaling regime where $A_{cl} \propto V_{cl}$. The growth just at the end of the plot is due to the largest cluster, which wraps around the lattice and merges with itself to form extra interior points. This plateau is the first indication that the surfaces are not smooth and are unstable towards the formation of quasi-one-dimensional objects. The observed proportionality of V_{cl} and A_{cl} is well known in the context of pure percolation in two and three dimensions [9]; to our knowledge it has not been measured for 3D Ising clusters. Note that in the well understood case of the 2D Ising model (which has a nonpathological continuum behavior) the cluster perimeter is not proportional to the area spanned by the cluster.

Turning to the analysis of the topology of the dual surfaces bounding the clusters, we consider the distribution $N_q(A)$, where g is the genus and A is the dual surface area. In Fig. 2, we present our data for genus 5 along with a best fit to the functional form

$$
N_q(A) = C_q A^{x(g)} e^{-\mu(g)A} . \tag{1}
$$

The fit is superb. One of our main results is that this functional form fits our data very well for $q > 2$ up to about $g = 20$ where our statistics become poor. The "cosmological constant" μ is found to be independent of the genus for $g > 2$ (Fig. 3). The value $\mu^{-1} = 114 \pm 3$ is proportional to the average surface area (in lattice units) per handle.

In Fig. 4 we plot the exponent $x(g)$ as a function of the genus. Once again after a transient region for small

FIG. 3. The dependence of the cosmological constant $\mu(g)$ on genus for FK clusters on the $L = 64$ bcc lattice at T_c .

genus $(g = 0 - 4)$ we find an almost linear behavior in the region $g = 5 - 15$ with a slope of 1.25 ± 0.1 . The deviations from linearity are small, and in our observation window they can be fitted with an effective exponent correction of order 0.1, or with logarithmic corrections. These make an estimate of the large genus behavior of $x(g)$ rather difficult. The region we are observing is still transitory, and we cannot exclude that the asymptotic slope of $x(g)$ could equal one at large g. This value would be expected if the handles were completely uncorrelated as for a Poisson distribution $P_g(A) = \frac{1}{g!}(\mu A)^g e$

The results presented above have also been analyzed for the simple cubic lattice. The data agree with those of the bcc lattice here and point to a good universal behavior. The main discrepancies can be traced to the short distance ambiguities which plague the definition of the dual surfaces on the simple cubic lattice. The scaling exponents are close for the two lattices. The difference among some nonuniversal quantities, e.g., $\mu^{-1} \sim 60$ on the simple cubic lattice, can be qualitatively understood from the ratio of the number of plaquettes of the respective Wigner-Seitz cells.

We will discuss in detail in [10) the analogous features both for the percolation of minority spins of the Ising model and for noninteracting bond percolation. The general picture is interestingly the same; indeed, the slope dx/dg for bond percolation is compatible with the value for FK clusters. However, the slope $dx/dg \sim 0.7 \pm 0.1$ in the range $q = 3 - 40$ for Ising minority spin percolation. The same caution as before applies to these slope values. Another interesting result is the similarity of the measured area scaling exponents ($\tau = 2.18 \pm 0.05$ upon

FIG. 4. The dependence of the exponent $x(g)$ (extracted from the fits by Eq. (I)] on genus for FK clusters on the $L = 64$ bcc lattice at T_c .

extrapolation to large lattices) as well as the linear relation between cluster volume and area at the respective critical points (FK clusters at T_c and minority spin clusters at T_n). The difference of the $x(g)$ estimated for the two interacting theories we are studying is interesting. It is possible that in the asymptotic region one will get 1.0 for the slope in both cases, but the large difference of the measured exponents (which are, on the contrary, very similar when looking at FK clusters and at bond percolation) says at least something about finite size corrections, i.e., about the nature of the interaction. Apart from this effect these results indicate that the cluster distribution scaling is rather insensitive to the average cluster density, which is about 10 times less for minority spin clusters. At least partially we may be observing some universality of diferent definitions of self-avoiding random surfaces.

We regard the outcome of our topological studies and the behavior $V_{\text{cl}} \sim A_{\text{cl}}$ as a strong indication that the cluster boundaries are in a "branched" phase. The topological evidence suggests that the surfaces grow fingers which reconnect with a fixed probability per unit area. The cosmological constant of the surfaces of fixed genus is nonzero at the critical point. Adjusting the temperature away from criticality will only increase μ , as the large surfaces are exponentially suppressed (apart from a few surfaces of the size of the lattice above the percolation threshold). Therefore there is no relevant parameter in the theory that could be tuned to allow large surfaces of low genus. One can imagine that some additional parameter (e.g., one that couples to the Euler density of the lattice surfaces, which depends on all the spins in a fundamental cell) could be fine-tuned to multicriticality (for another approach see [4]). Then there would be the possibility to have a scaling theory at fixed genus. However, Huse and Leibler [3] have argued that a phase transition to a droplet phase intervenes, in which the topological coupling favors breaking large surfaces into many tiny spheres.

Finally, in order to get a more accurate description of the geometry of the minority clusters, we analyzed two-dimensional slices of the lattice to obtain the distribution of cluster cross sections as a function of their perimeters. Below the *critical* temperature T_c the distribution drops off at a scale of the order of a few lattice spacings, providing further indication that the surfaces are composed of small, highly interconnected tubes. Remarkably, around T_c (recall that the surfaces have long since percolated at $T_p < T_c$) we find very good scaling behavior which must be entirely dominated by the cross sections of the large percolated cluster. Since one may view the percolated cluster as describing the Euclidean (transfer matrix) time evolution of interacting strings, one can observe the order-disorder transition of the Ising model directly in the properties of the string ensemble.

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