Large-cell Monte Carlo renormalization-group method for a new type of environmental percolation

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As a simple model for some diluted magnetic systems which present high percolation thresholds, we study a new type of environmental percolation model. In this model two neighboring magnetic sites are considered to be in the same cluster only if their nearest-neighbor sites in the same direction of the line joining them are also magnetic. By using a large-cell Monte Carlo renormalization-group method the percolation threshold in a square lattice is found to be $p_c = 0.741 \pm 0.002$ and the exponent for the correlation length $1/\nu = 0.75 \pm 0.02$, indicating that the model may be in the same universality class as the site percolation problem.

Percolation models play a fundamental role in the understanding of a variety of phenomena in physics.[1,2] Particularly interesting physical realizations of percolation phenomena are found in disordered magnetic systems. In these systems nonmagnetic ions replace magnetic ones in a random manner to produce clusters of magnetic sites of all sizes. Since for pure magnetic systems the critical temperature is a function of the exchange interaction, a decrease of the critical temperature is expected to follow the dilution of the magnetic atoms. The critical temperature reaches the limiting zero value at the percolation concentration of magnetic ions p_c. At $T=0$ the magnetic properties of the system will be entirely determined by the cluster distribution.

In the site percolation problem the magnetic ions correspond to occupied sites in a lattice and nonmagnetic ions to empty sites. Two neighboring magnetic ions are said to be in the same cluster regardless of the occupancy of the other neighboring sites. The percolation concentration for this model, obtained by numerical methods are for the square and cubic lattices $p_c = 0.5927 \pm 0.0001$ (Ref. 3) and $p_c = 0.3117 \pm 0.0002$ (Ref. 4), respectively.

Some diluted magnetic systems, however, appear to display a critical percolation concentration well above that predicted for the site percolation problem. In these systems, formation of a magnetic moment in a given magnetic ion can depend strongly on the local environment.[5] Thus, only magnetic sites with a given number of nearest-neighbor magnetic ions are included in a cluster.[6,7]

Recent[8,9] analysis of ^{19}F NMR linewidths in the randomly diluted magnetic system $KMn_pMg_{1-p}F_3$ and on its isostructural compound $KNi_pMg_{1-p}F_3$ show striking differences in their magnetic properties as a function of dilution. Experimental results for the percolation threshold in $KMn_pMg_{1-p}F_3$ yield a value consistent with the conventional site dilution model. However, the model appears to fail for $KNi_pMg_{1-p}F_3$ whose critical curve shows a tendency towards a higher percolation threshold. The above experimental results together with arguments on the nature of the exchange interaction between the Ni^{2+} ions for one compound and between the Mn^{2+} ions in the other led to the suggestion[8,9] that a model for $KNi_pMg_{1-p}F_3$ may be more realistic if one assumes that the exchange coupling between two nearest-neighbor Ni^{2+} ions depends on their surroundings in the following way: Two neighboring magnetic ions are considered members of the same magnetic cluster if their nearest neighbors along the line joining the two ions are also magnetic (see Fig. 1). In addition to predicting a higher percolation concentration, the model defined above could lead to a much larger linewidth in $KNi_pMg_{1-p}F_3$ for the same value of p suggesting a possible explanation for the absence of some of the ^{19}F NMR lines in this compound.[9]

The purpose of this work is to analyze the critical properties of the above described model near the percolation threshold by using renormalization-group techniques. For simplicity we shall restrict our analysis to square lattices.

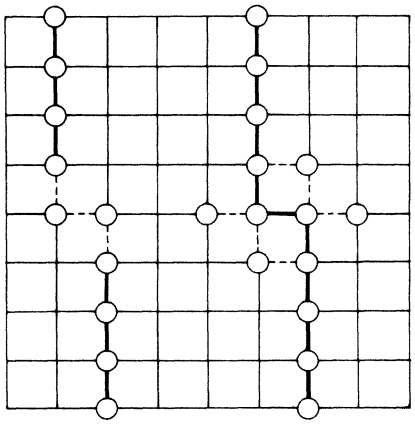

FIG. 1. The cluster on the left side of the figure is broken because sites along the line joining the atoms are empty in the region of the bend. The cluster on the right is not broken because of the environment of occupied sites around the bend.

To obtain the percolation concentration and the critical exponent ν for the correlation length we have applied the large-cell Monte Carlo renormalization-group (RG) method introduced by Reynolds, Stanley, and Klein,[10] which has provided reliable estimates for site and bond problems in two[10] and three[11] dimensions as well as in higher dimensions.[12] In this method we start partitioning the lattice into cells that cover the entire lattice and have precisely its symmetry. Each cell now is replaced by a site whose probability of being occupied depends on the cell size and of the fraction p of the magnetic sites randomly distributed in the lattice. The renormalized site occupation is defined as the total probability $p'=R(b,p)$ in which a cell of size b containing b^d sites percolates (a two-dimensional cell percolates if a connected path of occupied sites exists which spans the cell from top to bottom) at a given concentration p. This procedure defines a renormalization-group transformation $p'=R(p)$, where $p^*=R(p^*)$ is the fixed-point equation. One should emphasize that, to avoid proliferation of probabilities in the renormalization-group transformation, the connectivity between distant cells is neglected. However, as one increases the cell size this interface effect becomes progressively small.[10] The linearization of the RG transformation about the fixed point provides the thermal scaling power $y_t=1/\nu$ through the relation,

$$y_t=\frac{\ln b}{\ln\lambda} , \tag{1a}$$

where

$$\lambda=\left.\frac{dR}{dp}\right|_{p^*} . \tag{1b}$$

This approach can be applied exactly for cells of small sizes. In the present model for $b=3$, the exact recursion relation $p'=R(p)$ reads as

$$p'=p^9+9p^8q+36p^7q^2+57p^6q^3 +45p^5q^4+18p^4q^5+3p^3q^6 , \tag{2}$$

with $q=1-p$. The corresponding nontrivial fixed point and thermal exponent are, respectively, $p^*=0.682$ and $y_t=0.605$. This is, however, a crude estimate for these critical parameters since the independent-cell approximation fails for small b. To obtain better results one should rely on larger cells. However, since it is not feasible to calculate the recursion relation in closed form we shall evaluate it in a quite accurate way by using Monte Carlo simulations.

The recursion relation is numerically found by constructing a histogram for the density probability $L(p)$, that is, $L(p)dp$ represents the probability for the cell to percolate in the interval $[p,p+dp]$. Hence the site occupation probability which renormalizes a cell at concentration p is given by

$$p'=R(p)=\int L(p)dp . \tag{3}$$

From numerical results, the density probability $L(p)$ shows a peak near the average percolation threshold $\langle p\rangle$. Finite-size scaling also predicts that for large b the $\langle p\rangle$ approaches the asymptotic value p_c for the infinite system as $\langle p\rangle-p_c\sim b^{-1/\nu}$. Moreover, the width $\sigma^2\equiv\langle p^2\rangle-\langle p\rangle^2$ of $L(p)$ also behaves for large b as $\sigma\sim b^{-1/\nu}$ and fits a Gaussian distribution:

$$L(p)=(2\pi\sigma^2)^{-1/2}\exp[-(p-\langle p\rangle)^2/2\sigma^2], \ (b\to\infty) . \tag{4}$$

We have approximated the maximum of $L(p)$ by $\langle p\rangle$ which by its turn, for large b, may be identified with the fixed point p^*. By using (1) and (3), one can relate the thermal exponent y_t, with the width of the Gaussian distribution σ, through

$$y_t=\ln(2\pi\sigma^2)^{-1/2}/\ln b, \ (b\to\infty) . \tag{5}$$

Our results are shown in Table I for a sequence of increasing cell sizes up to $b=250$. The second column represents the number of cells of size b used to obtain the average value of the percolation threshold $\langle p_c(b)\rangle$ and the

TABLE I. Environmental percolation (square lattice).

Cell size (b)	Trials	$\langle p_c\rangle$	$(\langle p_c^2\rangle-\langle p_c\rangle^2)^{1/2}$	$1/\nu$
3	Exact	0.578571	0.182857	0.60530
3	100000	0.578758	0.182855	0.71009
10	50000	0.702699	0.081640	0.68900
20	40000	0.727432	0.047100	0.71319
30	30000	0.733072	0.034456	0.72008
40	30000	0.735785	0.027813	0.72198
50	10000	0.736941	0.023386	0.72511
60	10000	0.737475	0.020356	0.72672
70	8000	0.738215	0.018419	0.72388
80	8000	0.738476	0.016421	0.72803
100	8000	0.738859	0.013970	0.72785
120	6000	0.739033	0.012311	0.72654
150	4000	0.739346	0.010229	0.73116
200	2000	0.739216	0.008401	0.72862
250	2000	0.739459	0.007034	0.73135

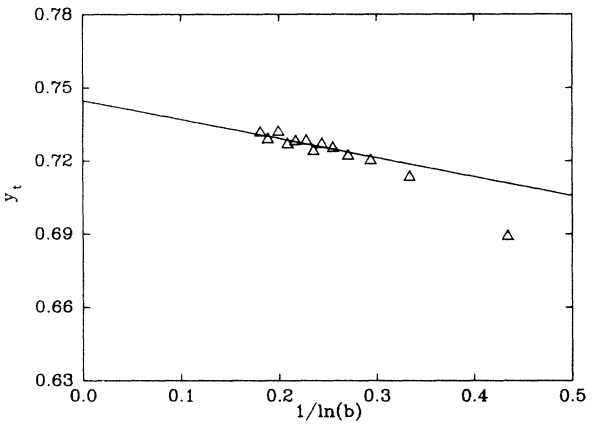

FIG. 2. Results for the dependence of the thermal exponent $y_t(b)$ with the size cell b. The intercept gives the estimate for the infinite square lattice.

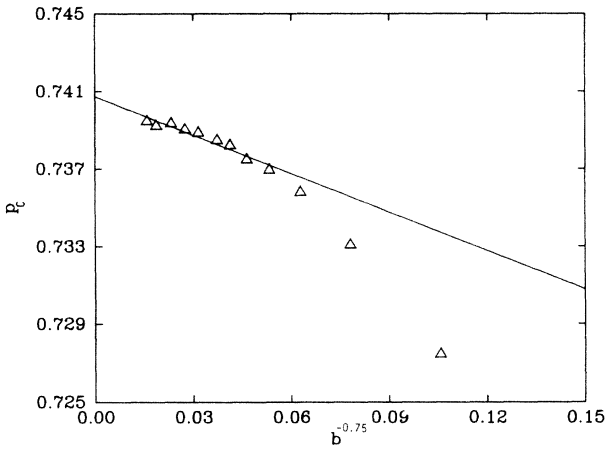

FIG. 3. Average percolation threshold $p_c(b)$ vs b^{-y_t}. The trial value for y_t was chosen to be 0.75. The intercept gives the estimate for the percolation concentration for the infinite square lattice.

width σ of density probability $L(p)$. The thermal exponent $y_t = 1/\nu$ has been calculated from (5) by assuming a Gaussian distribution for the probability density $L(p)$ independent of the cell size. The numerical calculation for $b=3$ has been performed for the purpose of checking our computer program. The discrepancy between exact and numerical estimates for the thermal exponent $1/\nu$ reflects the fact that the Gaussian approximation fails for small size cells. Extrapolation of the data to the limit $b \rightarrow \infty$ by using a least-squares fit of the data points in the interval $50 \leq b \leq 250$ are shown in Figs. 2 and 3. In Fig. 2 we present the results for the dependence of the thermal exponent y_t with the cell size. Extrapolation for infinite b gives $y_t = 0.75 \pm 0.02$, which is consistent with the conventional percolation problem. By assuming the conjectured exact value for the thermal exponent $y_t = \frac{3}{4}$ we obtain for the extrapolated percolation concentration $p_c = 0.741 \pm 0.002$, which is substantially larger than that found for the conventional percolation problem.

To conclude, we have studied a new type of environmental percolation problem which may be useful to model some dilute magnetic systems which present high percolation thresholds. Monte Carlo analysis of these dilute magnetic systems for finite temperature will be presented elsewhere.

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